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TO: Rei-Tsang Shiao **Location: 5a10 / 5c18** **Monday, March 14, 2005** **Art Unit: 1626** **Phone: 571-272-0707** **Serial Number: 10 / 622130**	**From: Jan Delaval** **Location: Biotech-Chem Library** **Remsen 1a51** **Phone: 571-272-22504** **jan.delaval@uspto.gov**

Search Notes

Access DB# 146707

Ian Boland for search

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Robert (Rex) Shiao Examiner #: 79521 Date: 3/3/05

Art Unit: 1626 Phone Number 2-0907 Serial Number: 10/622,430

Mail Box and Bldg/Room Location: 5A10/5C18 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

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Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

* any question please call me at 2-0907

Title of invention: Heterodiamondoids

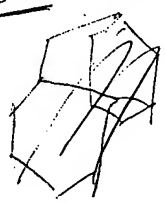
Inventors (please provide full names): Liu et al

Earliest Priority Filing Date: _____

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

I search a heterodiamondoid compound have a diamondoid nucleus selected from trimantane or tetramantane nucleus, and the nucleus has a atom selected from N, S, O (see Fig 1, 5, 6, 7, 8)

II Second compound (see Fig 2), of the ring structure and one of carbon atom is replaced by N, O, S, Se, B, P, As



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STAFF USE ONLY

Searcher: _____

Searcher Phone #: 272-04

Searcher Location: _____

Date Searcher Picked Up: 3/10/05

Date Completed: 3/14/05

Searcher Prep & Review Time: _____

Clerical Prep Time: 30

Online Time: + 90

Type of Search

NA Sequence (#) _____

AA Sequence (#) _____

Structure (#) ✓

Bibliographic _____

Litigation _____

Fulltext _____

Patent Family _____

Other _____

Vendors and cost where applicable

STN ✓

Dialog _____

Questel/Orbit _____

Dr.Link _____

Lexis/Nexis _____

Sequence Systems _____

WWW/Internet _____

Other (specify) _____

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               E CHEVRON/PA,CS
L3          5478 S CHEVRON?/PA,CS
               E CHEVRO/PA,CS
               E LIU S/AU
L4           528 S E3,E12
               E LIU SHENG/AU
L5           148 S E3,E16
               E LIU SHENGGAO/AU
L6            22 S E3
               E CARLSON R/AU
L7            88 S E3,E17,E18
               E CARLSON ROB/AU
L8           163 S E4,E21-E25
               E DAHL J/AU
L9            24 S E3,E7,E8
               E DAHL JEREMY/AU
L10           32 S E3-E7
L11           77 S ?TETRAMANTAN? OR ?TRIAMANTAN?
L12          263 S ?DIAMONDOID?
L13            3 S L1,L3-L10 AND L2
L14           21 S L1,L3-L10 AND L11,L12
L15           21 S L13,L14
L16            5 S L15 AND ?ADAMANTAN?
L17           13 S L15 AND ?AMANTAN?
L18           13 S L16,L17
L19            8 S L15 NOT L18
L20           41 S L15-L19,L2
L21           37 S L12 AND L11
L22           98 S L12 AND ?AMANTAN?
L23           98 S L21,L22

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L28            80 S L27 AND ?AMANTAN?/CNS
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L30            38 S L29 AND (SE OR AS OR B OR AL OR SI OR N OR P OR O OR S)/ELS
L31            16 S L30 AND (C15H20O2 OR C16H20O4 OR C14H20O OR C18H22O OR C18H26
L32            22 S L30 NOT L31
L33            42 S L28 NOT L30
L34           279 S L27 NOT L28-L33
L35             0 S L34 AND ?MANTAN?/CNS
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L39             5 S L38 AND (CARBOXYLIC OR C21H26O)
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     FILE 'USPATFULL' ENTERED AT 10:23:27 ON 10 MAR 2005
L65           1 S L44

=> fil uspatful
FILE 'USPATFULL' ENTERED AT 10:23:48 ON 10 MAR 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 8 Mar 2005 (20050308/PD)
FILE LAST UPDATED: 8 Mar 2005 (20050308/ED)
HIGHEST GRANTED PATENT NUMBER: US6865747
HIGHEST APPLICATION PUBLICATION NUMBER: US2005050605
CA INDEXING IS CURRENT THROUGH 8 Mar 2005 (20050308/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 8 Mar 2005 (20050308/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2005

>>>  USPAT2 is now available.  USPATFULL contains full text of the     <<<
>>>  original, i.e., the earliest published granted patents or         <<<
>>>  applications.  USPAT2 contains full text of the latest US         <<<
>>>  publications, starting in 2001, for the inventions covered in     <<<
>>>  USPATFULL.  A USPATFULL record contains not only the original     <<<
>>>  published document but also a list of any subsequent              <<<
>>>  publications.  The publication number, patent kind code, and      <<<
>>>  publication date for all the US publications for an invention     <<<
>>>  are displayed in the PI (Patent Information) field of USPATFULL   <<<
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>>>  /PK, etc.                                                         <<<

>>>  USPATFULL and USPAT2 can be accessed and searched together        <<<
>>>  through the new cluster USPATALL.  Type FILE USPATALL to          <<<
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>>> enter this cluster. <<<
>>> <<<
>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l65 bib abs hitstr

L65 ANSWER 1 OF 1 USPATFULL on STN
AN 2004:77366 USPATFULL
TI Heterodiamondoids
IN Liu, Shenggao, Hercules, CA, UNITED STATES
Carlson, Robert M., Petaluma, CA, UNITED STATES
Dahl, Jeremy E., Palo Alto, CA, UNITED STATES
PA CHEVRON USA INC. (U.S. corporation)
PI US 2004059145 A1 20040325
AI US 2003-622130 A1 20030716 (10)
PRAI US 2002-397367P 20020718 (60)
DT Utility
FS APPLICATION
LREP William H. Benz, BURNS, DOANE, SWECKER & MATHIS, L.L.P., P.O. Box 1404, Alexandria, VA, 22313-1404
CLMN Number of Claims: 37
ECL Exemplary Claim: 1
DRWN 51 Drawing Page(s)
LN.CNT 2469
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB This invention is related to heteroatom containing diamondoids (i.e., "heterodiamondoids") which are compounds having a diamondoid nucleus in which one or more of the diamondoid nucleus carbons has been substitutionally replaced with a noncarbon atom. These heteroatom substituents impart desirable properties to the diamondoid. In addition, the heterodiamondoids are functionalized affording compounds carrying one or more functional groups covalently pendant therefrom. This invention is further related to polymerizable functionalized heterodiamondoids. In a preferred aspect of this invention the diamondoid nuclei are triamantane and higher diamondoid nuclei. In another preferred aspect, the heteroatoms are selected to give rise to diamondoid materials which can serve as n- and p-type materials in electronic devices can serve as optically active materials.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **652998-90-8**, [121212121] Oxadecamantane **652998-91-9**, [121212121] Thiadecamantane **652998-92-0**, [121212121] Selenadecamantane **652998-93-1**, [121212121] Boradecamantane **652998-94-2**, [121212121] Azadecamantane **652998-95-3**, [121212121] Phosphadecamantane **652998-96-4**, [121212121] Arsadecamantane **652998-98-6**, [1212121212] Oxaundecamantane **652998-99-7**, [1212121212] Thiaundecamantane **652999-00-3**, [1212121212] Selenaundecamantane **652999-01-4**, [1212121212] Boraundecamantane **652999-02-5**, [1212121212] Azaundecamantane **652999-03-6**, [1212121212] Phosphaundecamantane **652999-04-7**, [1212121212] Arsaundecamantane **652999-05-8** **652999-06-9** **652999-08-1** **652999-09-2** **652999-11-6** **652999-12-7** **652999-35-4** **652999-36-5** **652999-38-7** **652999-39-8** **652999-40-1**, [121212121] Boradecamantane **652999-41-2**, [121212121] Azadecamantane **652999-42-3**, [121212121] Phosphadecamantane **652999-43-4**, [121212121] Arsadecamantane **652999-44-5**, [1212121212] Boraundecamantane **652999-45-6**

, [1212121212] Azaundecamantane **652999-46-7**, [1212121212] Phosphaundecamantane **652999-47-8**, [1212121212] Arsaundecamantane
(calcn. of heat of formation; preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

RN 652998-90-8 USPATFULL
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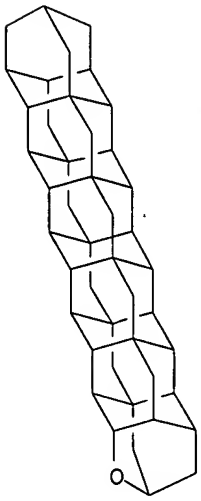

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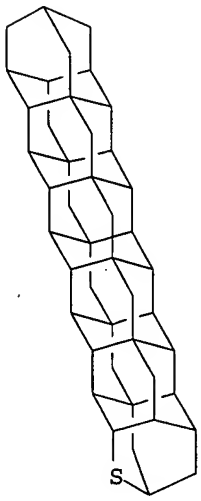

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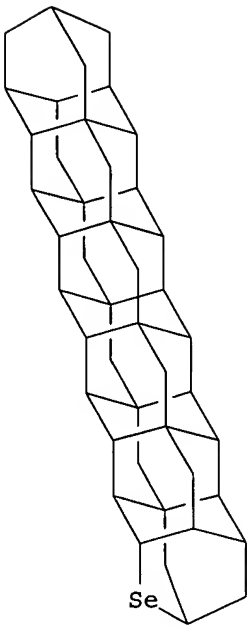

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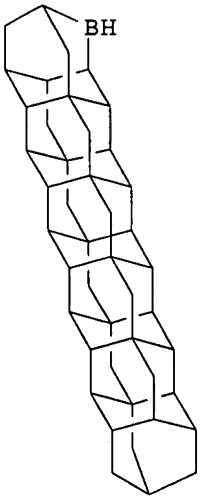

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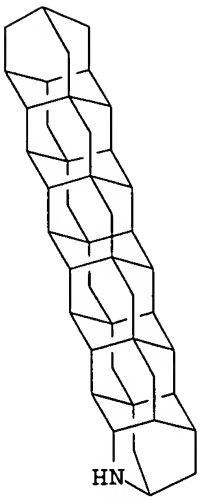

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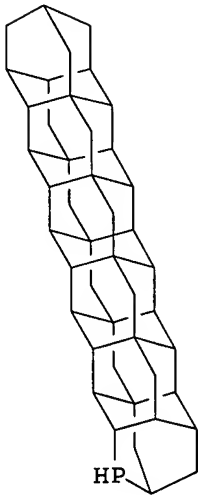

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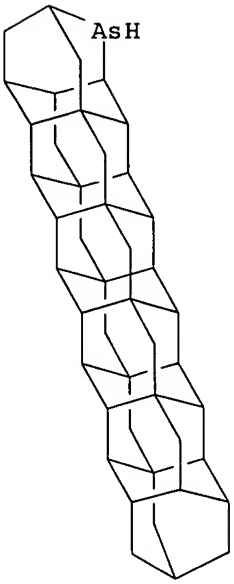

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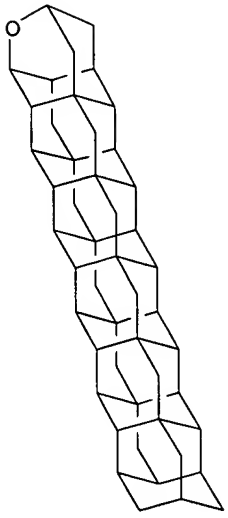

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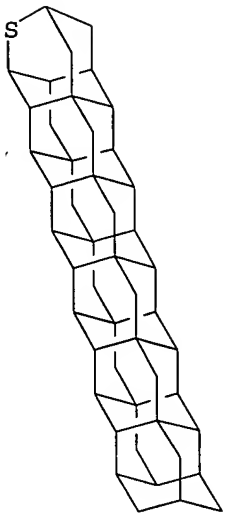

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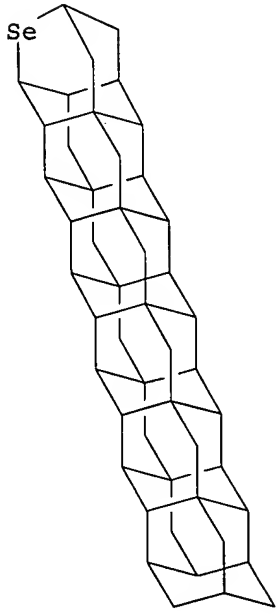

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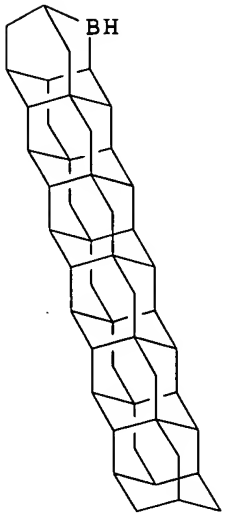

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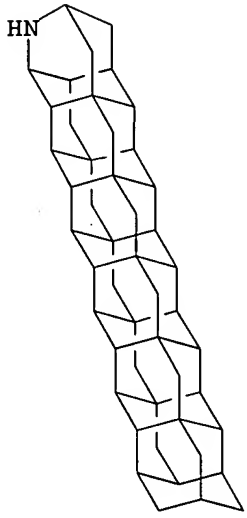

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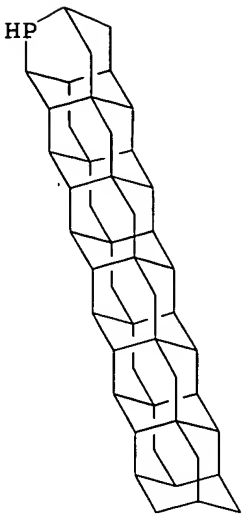

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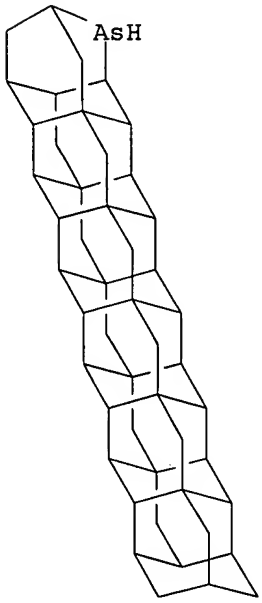

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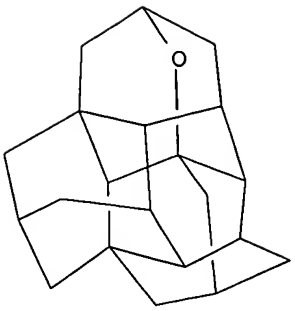

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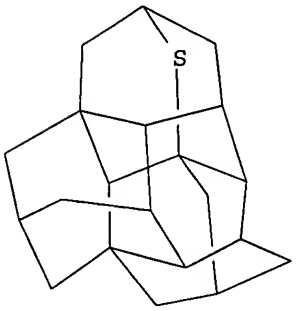

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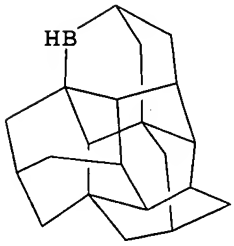

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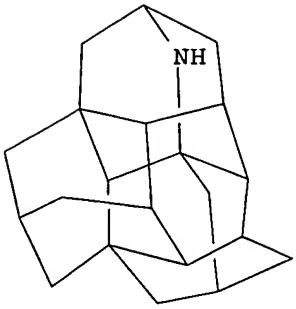

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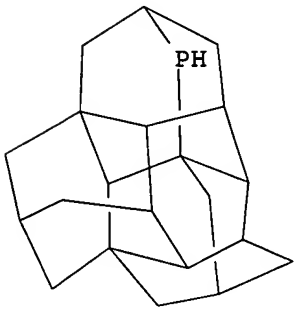

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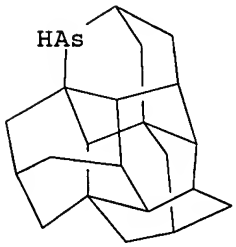

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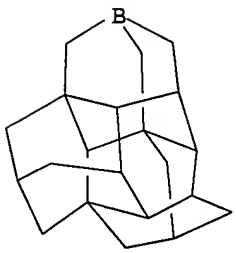

RN 652999-36-5 USPATFULL
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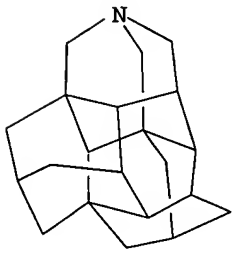
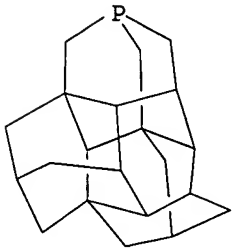
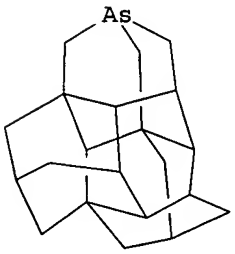


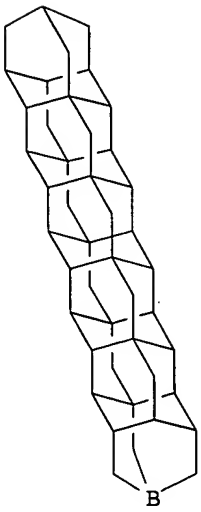
RN 652999-38-7 USPATFULL
CN 3H,4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenz[de,h]isophosphinoline, decahydro- (9CI) (CA INDEX NAME)



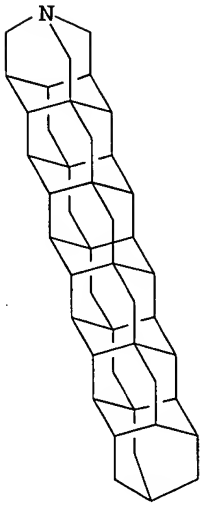
RN 652999-39-8 USPATFULL
CN 3H,4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenz[de,h]isoarsinoline, decahydro- (9CI) (CA INDEX NAME)



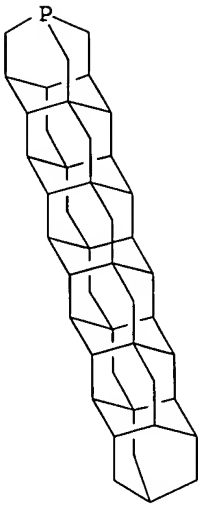
RN 652999-40-1 USPATFULL
CN [121212121] Boradecamantane (9CI) (CA INDEX NAME)



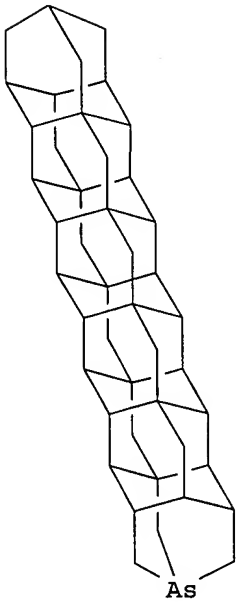
RN 652999-41-2 USPATFULL
CN [121212121] Azadecamantane (9CI) (CA INDEX NAME)



RN 652999-42-3 USPATFULL
CN [121212121] Phosphadecamantane (9CI) (CA INDEX NAME)

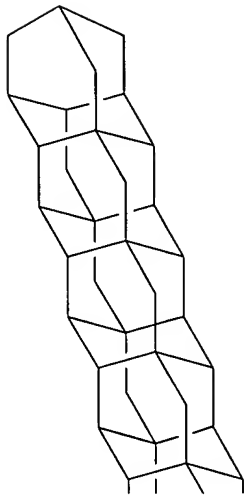


RN 652999-43-4 USPATFULL
CN [121212121] Arsadecamantane (9CI) (CA INDEX NAME)

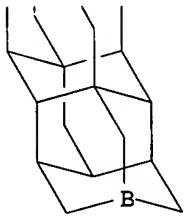


RN 652999-44-5 USPATFULL
CN [1212121212] Boraundecamantane (9CI) (CA INDEX NAME)

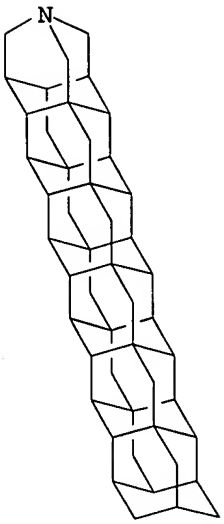
PAGE 1-A



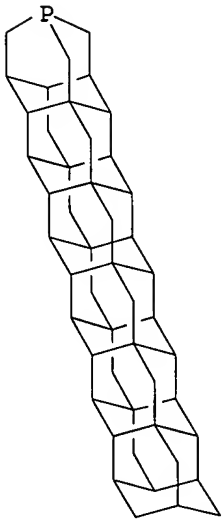
PAGE 2-A



RN 652999-45-6 USPATFULL
CN [1212121212] Azaundecamantane (9CI) (CA INDEX NAME)

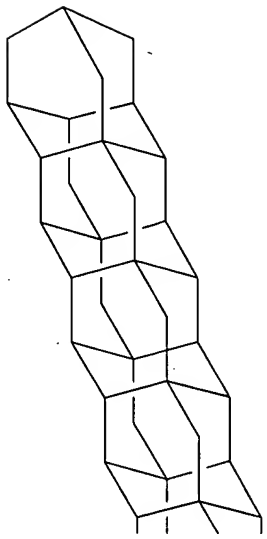


RN 652999-46-7 USPATFULL
CN [1212121212] Phosphaundecamantane (9CI) (CA INDEX NAME)

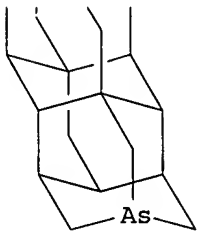


RN 652999-47-8 USPATFULL
CN [1212121212] Arsaundecamantane (9CI) (CA INDEX NAME)

PAGE 1-A



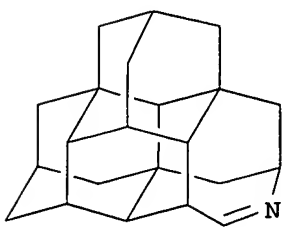
PAGE 2-A



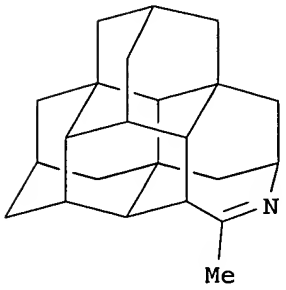
IT **652999-16-1P 652999-17-2P 652999-18-3P**
652999-19-4P 652999-20-7P 652999-23-0P
652999-24-1P 652999-25-2P
(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

RN 652999-16-1 USPATFULL

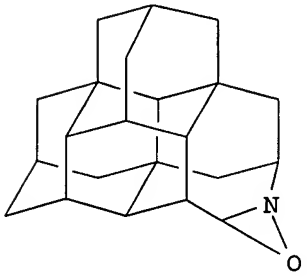
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylideneanthra[9,1-cd]azepine, 3,4,6,7,7a,8a,9,10,11,12a,12b,12c-dodecahydro- (9CI) (CA INDEX NAME)



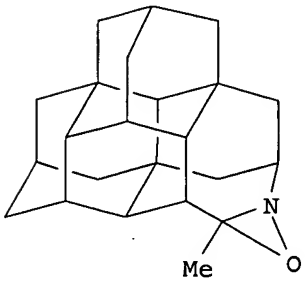
RN 652999-17-2 USPATFULL
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylideneanthra[9,1-cd]azepine, 3,4,6,7,7a,8a,9,10,11,12a,12b,12c-dodecahydro-1-methyl- (9CI) (CA INDEX NAME)



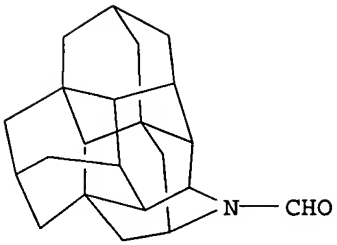
RN 652999-18-3 USPATFULL
CN 8H,9H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-5H-anthra[9,1-cd]oxazirino[2,3-a]azepine, dodecahydro- (9CI) (CA INDEX NAME)



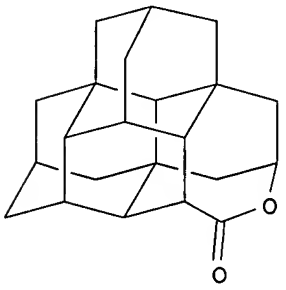
RN 652999-19-4 USPATFULL
CN 8H,9H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-5H-anthra[9,1-cd]oxazirino[2,3-a]azepine, dodecahydro-12c-methyl- (9CI) (CA INDEX NAME)



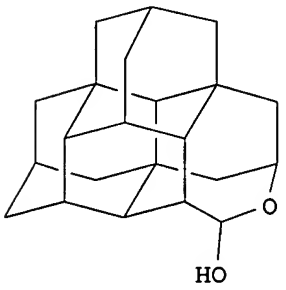
RN 652999-20-7 USPATFULL
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenzo[de,h]quinoline-1-carboxaldehyde, dodecahydro- (9CI) (CA INDEX NAME)



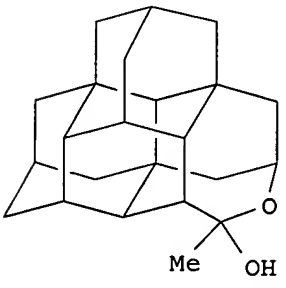
RN 652999-23-0 USPATFULL
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-one, dodecahydro- (9CI) (CA INDEX NAME)



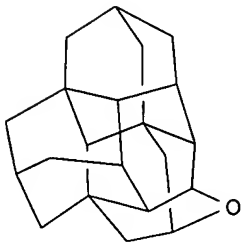
RN 652999-24-1 USPATFULL
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-ol, dodecahydro- (9CI) (CA INDEX NAME)



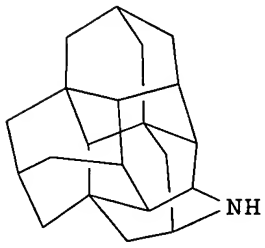
RN 652999-25-2 USPATFULL
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-ol, dodecahydro-1-methyl- (9CI) (CA INDEX NAME)



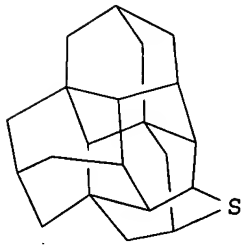
IT **652999-15-0P 652999-21-8P 652999-32-1P**
(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)
RN 652999-15-0 USPATFULL
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]pyran, dodecahydro- (9CI) (CA INDEX NAME)



RN 652999-21-8 USPATFULL
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenzo[de,h]quinoline, dodecahydro- (9CI) (CA INDEX NAME)



RN 652999-32-1 USPATFULL
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]thiopyran, dodecahydro- (9CI) (CA INDEX NAME)



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FILE LAST UPDATED: 9 Mar 2005 (20050309/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L64 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:641668 HCAPLUS
DN 141:320341
ED Entered STN: 10 Aug 2004
TI Diamond fragments as building blocks of functional nanostructures
AU McIntosh, Gregory C.; Yoon, Mina; Berber, Savas; Tomanek, David
CS Naval Base, Defence Technology Agency, Auckland, N. Z.
SO Physical Review B: Condensed Matter and Materials Physics (2004), 70(4), 045401/1-045401/8
CODEN: PRBMDO; ISSN: 0163-1829
PB American Physical Society
DT Journal
LA English
CC 65-3 (General Physical Chemistry)
AB Using d. functional theory, we investigate the equilibrium structure, stability, and electronic properties of nanostructured, hydrogen-terminated diamond fragments. The equilibrium atomic arrangement and electronic structure of these nanostructures turn out to be very similar to bulk diamond. We find that such **diamondoids** may enter spontaneously into carbon nanotubes. Polymerization inside a nanotube is favored especially when boron and nitrogen are substituted for carbon atoms.
ST **diamondoid** nanostructure electronic structure stability
IT LUMO (molecular orbital)
(HOMO gap; diamond fragments as building blocks of functional nanostructures studied by DFT)
IT HOMO (molecular orbital)
(LUMO gap; diamond fragments as building blocks of functional nanostructures studied by DFT)
IT Bond length
(carbon-carbon; diamond fragments as building blocks of functional nanostructures studied by DFT)
IT Nanotubes
(carbon; diamond fragments as building blocks of functional nanostructures studied by DFT)
IT Band gap
Band structure
Binding energy
Cluster model
Conduction band
Density of states
Electron density
HOMO (molecular orbital)
LUMO (molecular orbital)
Nanostructures
Polymerization
Valence band

(diamond fragments as building blocks of functional nanostructures studied by DFT)
IT Energy
(formation; diamond fragments as building blocks of functional nanostructures studied by DFT)
IT 281-23-2, **Adamantane** 2292-79-7, **Diamantane**
7782-40-3, Diamond, properties 27745-90-0, **Tetramantane**
112761-65-6, **Decamantane 765943-15-5**
765943-16-6
RL: PRP (Properties)
(diamond fragments as building blocks of functional nanostructures studied by DFT)
RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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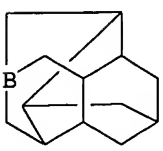
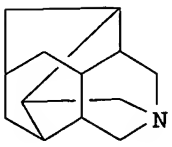
IT **765943-15-5 765943-16-6**
RL: PRP (Properties)
(diamond fragments as building blocks of functional nanostructures studied by DFT)
RN 765943-15-5 HCAPLUS
CN 1H-2,8,4,6-[1,2,3,4]Butanetetrayl-2-benzoborin, octahydro- (9CI) (CA INDEX NAME)



RN 765943-16-6 HCAPLUS
CN 1H-2,8,4,6-[1,2,3,4]Butanetetraylisoquinoline, octahydro- (9CI) (CA INDEX

NAME)



L64 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:365485 HCAPLUS
DN 141:318401
ED Entered STN: 05 May 2004
TI Theoretical analysis of diamond mechanosynthesis. Part II. C2 mediated growth of diamond C(110) surface via Si/Ge-triadamantane dimer placement tools
AU Mann, David J.; Peng, Jingping; Freitas, Robert A., Jr.; Merkle, Ralph C.
CS Zyvex Corp., Richardson, TX, 75081, USA
SO Journal of Computational and Theoretical Nanoscience (2004), 1(1), 71-80
CODEN: JCTNAB; ISSN: 1546-1955
PB American Scientific Publishers
DT Journal
LA English
CC 57-8 (Ceramics)
Section cross-reference(s): 66, 75
AB This paper presents a computational and theor. investigation of the vacuum mechanosynthesis of diamond on the clean C(110) surface from carbon dimer (C2) precursors positionally constrained throughout the reaction pathway by silicon- or germanium-doped triadamantane derivs. mounted on a scanning probe tip. Interactions between the dimer placement tools and the bare diamond C(110) surface are investigated using D. Functional Theory (DFT) with generalized gradient approximation (GGA) by constructing the reaction path potential energy profiles and analyzing ab initio mol. dynamics simulations. Similar methods are applied to study the energetics and kinetics of recharging the tool with acetylene. Mol. mechanics simulations on extended tool tips are carried out to elucidate the positional uncertainty of the carbon dimer due to thermal fluctuations, and the possibility of intermol. dimerization and dehydrogenation of the dimer placement tools is explored.
ST diamond growth dicarbon precursor
IT Simulation and Modeling, physicochemical
(mol. dynamics; theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)
IT Reaction mechanism
(surface; theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)
IT Mechanochemical reaction
Surface structure
(theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)
IT 7782-40-3, Diamond, processes
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)
IT **681029-68-5 681029-69-6**
RL: PRP (Properties)

(theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)

IT 12070-15-4, Carbon dimer
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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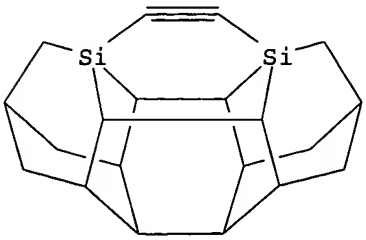
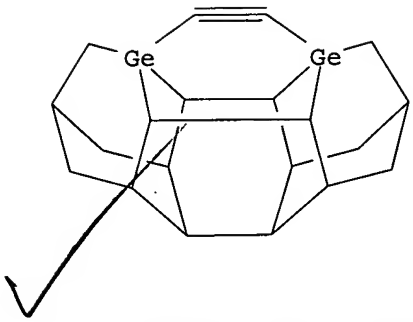
(25) van Zandt, W; J Am Chem Soc 1966, V88, P3862
(26) Von Schleyer, P; J Am Chem Soc 1957, V79, P3292

IT **681029-68-5 681029-69-6**
RL: PRP (Properties)
(theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)

RN 681029-68-5 HCAPLUS
CN Disila[6]fulleroid-C22, tetradehydro- (9CI) (CA INDEX NAME)



RN 681029-69-6 HCAPLUS
CN Digerma[6]fulleroid-C22, tetradehydro- (9CI) (CA INDEX NAME)



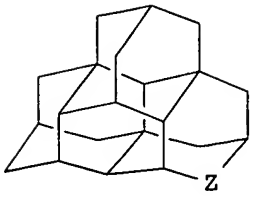
L64 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:80675 HCAPLUS
DN 140:146009
ED Entered STN: 01 Feb 2004
TI Preparation of **heterodiamondoids** from fused **adamantanes**
IN **Liu, Shenggao; Carlson, Robert M.**
PA **Chevron U.S.A. Inc., USA**; Dahl, Jeremy E.
SO PCT Int. Appl., 134 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D311-78
ICS C07D313-06; C07D335-04; C07D221-18
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 76
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004009577	A1	20040129	WO 2003-US22483	20030717 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004059145	A1	20040325	US 2003-622130	20030716 <--
PRAI	US 2002-397367P	P	20020718 <--		
	US 2002-397368P	P	20020718		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004009577	ICM	C07D311-78
	ICS	C07D313-06; C07D335-04; C07D221-18
US 2004059145	ECLA	C07C023/20; C07C049/423; C07C049/617; C07C061/29; C07D221/22; C07D311/96; C07D313/06; C07D335/04; C07D471/10+221C+221C+9; C07F009/6568C <--

OS MARPAT 140:146009
GI



I

AB This invention is related to heteroatom containing **diamondoids** (i.e., '**heterodiamondoids**'), e.g. **azatetramantane**, **oxatetramantane**, and **thiatetramantane** (I; X = NH, O, S), which are compds. having a **diamondoid** nucleus in which one or more of the **diamondoid** nucleus carbons has been substitutionally replaced with a noncarbon atom. These heteroatom substituents impart desirable properties to the **diamondoid.** In addition, the **heterodiamondoids** are functionalized affording compds. carrying one or more functional groups covalently pendant therefrom. This invention is further related to polymerizable functionalized **heterodiamondoids.** In a preferred aspect of this invention the **diamondoid** nuclei are **triamantane** and higher **diamondoid** nuclei. In another preferred aspect, the heteroatoms are selected to give rise to **diamondoid** materials which can serve as n- and p-type materials in electronic devices and in optical devices as optically active materials (no data).

ST **heterodiamondoid** prepn; **azatetramantane** **oxatetramantane** **thiatetramantane** prepn

IT Formation enthalpy
(preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)

IT Heterocyclic compounds
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)

IT 652998-89-5, [121212121] **Decamantane 652998-90-8**, [121212121] **Oxadecamantane 652998-91-9**, [121212121] **Thiadecamantane 652998-92-0**, [121212121] **Selenadecamantane 652998-93-1**, [121212121] **Boradecamantane 652998-94-2**, [121212121] **Azadecamantane 652998-95-3**, [121212121] **Phosphadecamantane 652998-96-4**, [121212121] **Arsadecamantane** 652998-97-5, [1212121212] **Undecamantane 652998-98-6**, [1212121212] **Oxaundecamantane 652998-99-7**, [1212121212] **Thiaundecamantane 652999-00-3**, [1212121212] **Selenaundecamantane 652999-01-4**, [1212121212] **Boraundecamantane 652999-02-5**, [1212121212] **Azaundecamantane 652999-03-6**, [1212121212] **Phosphaundecamantane 652999-04-7**, [1212121212] **Arsaundecamantane 652999-05-8 652999-06-9** 652999-07-0 **652999-08-1 652999-09-2 652999-11-6 652999-12-7 652999-35-4 652999-36-5 652999-38-7 652999-39-8 652999-40-1**, [121212121] **Boradecamantane 652999-41-2**, [121212121] **Azadecamantane 652999-42-3**, [121212121] **Phosphadecamantane 652999-43-4**, [121212121] **Arsadecamantane 652999-44-5**, [1212121212] **Boraundecamantane 652999-45-6**, [1212121212] **Azaundecamantane 652999-46-7**, [1212121212]

Phosphaundecamantane 652999-47-8, [1212121212]
Arsaundecamantane
RL: PRP (Properties)
(calcn. of heat of formation; preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)

IT 917-54-4, Methyllithium 27745-90-0 73635-95-7 73635-96-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)

IT 546101-72-8P 546102-13-0P 652999-13-8P 652999-14-9P
652999-16-1P 652999-17-2P 652999-18-3P
652999-19-4P 652999-20-7P 652999-23-0P
652999-24-1P 652999-25-2P 652999-26-3P 652999-27-4P
652999-29-6P 652999-30-9P 652999-31-0P 652999-33-2P 652999-34-3P
653570-14-0P 653570-15-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)

IT **652999-15-0P 652999-21-8P** 652999-22-9P 652999-28-5P
652999-32-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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(3) Dahl, J; WO 02058139 A 2002 HCAPLUS
(4) Dahl, J; WO 03050066 A 2003 HCAPLUS
(5) Fritz, G; ANGEWANDTE CHEMIE, INTERNATIONAL EDITION IN ENGLISH 1970, V9(6), P464 HCAPLUS
(6) Fritz, G; ZEITSCHRIFT FUER ANORGANISCHE UND ALLGEMEINE CHEMIE 1984, V512, P103 HCAPLUS
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(8) Mobil Oil Corp; WO 9506019 A 1995 HCAPLUS
(9) Mochizuki, Y; CHEMICAL PHYSICS LETTERS 2001, V336(5,6), P451 HCAPLUS

IT **652998-90-8**, [121212121] **Oxadecamantane**
652998-91-9, [121212121] **Thiadecamantane**
652998-92-0, [121212121] **Selenadecamantane**
652998-93-1, [121212121] **Boradecamantane**
652998-94-2, [121212121] **Azadecamantane**
652998-95-3, [121212121] **Phosphadecamantane**
652998-96-4, [121212121] **Arsadecamantane**
652998-98-6, [1212121212] **Oxaundecamantane**
652998-99-7, [1212121212] **Thiaundecamantane**
652999-00-3, [1212121212] **Selenaundecamantane**
652999-01-4, [1212121212] **Boraundecamantane**
652999-02-5, [1212121212] **Azaundecamantane**
652999-03-6, [1212121212] **Phosphaundecamantane**
652999-04-7, [1212121212] **Arsaundecamantane**
652999-05-8 652999-06-9 652999-08-1
652999-09-2 652999-11-6 652999-12-7
652999-35-4 652999-36-5 652999-38-7
652999-39-8 652999-40-1, [121212121]
Boradecamantane 652999-41-2, [121212121]
Azadecamantane 652999-42-3, [121212121]
Phosphadecamantane 652999-43-4, [121212121]
Arsadecamantane 652999-44-5, [1212121212]

Boraundecamantane 652999-45-6, [1212121212]
Azaundecamantane 652999-46-7, [1212121212]
Phosphaundecamantane 652999-47-8, [1212121212]
Arsaundecamantane
RL: PRP (Properties)
(calcn. of heat of formation; preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)

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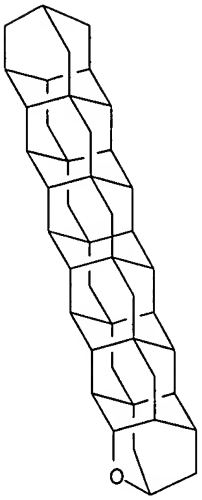

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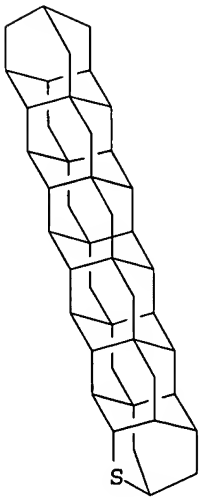

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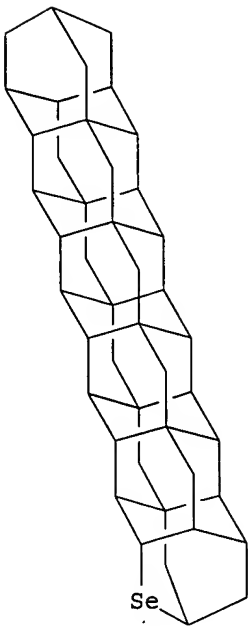

RN 652998-93-1 HCAPLUS
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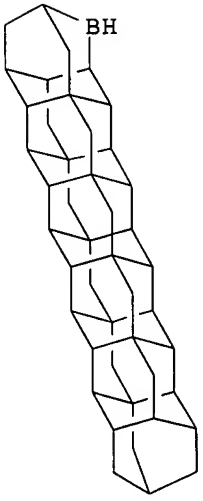

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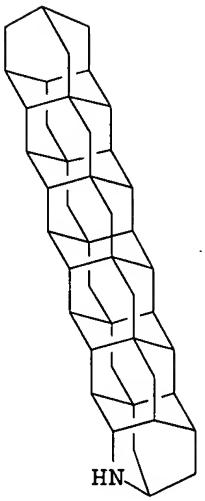

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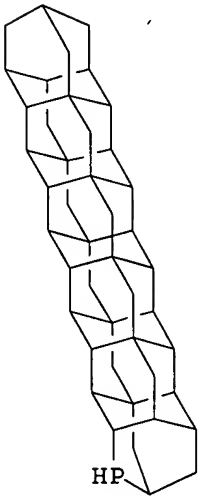

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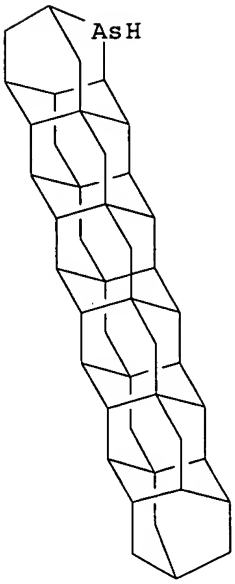

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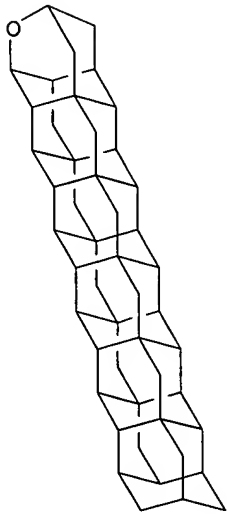

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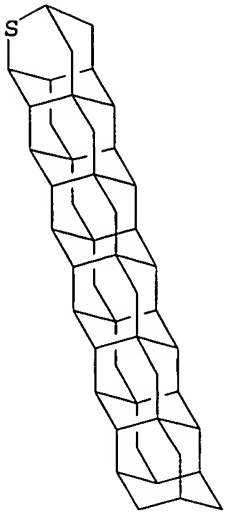

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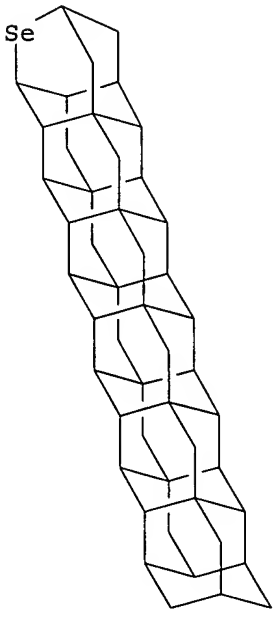

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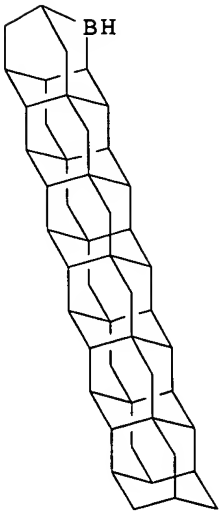

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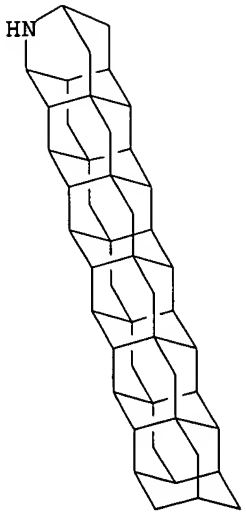

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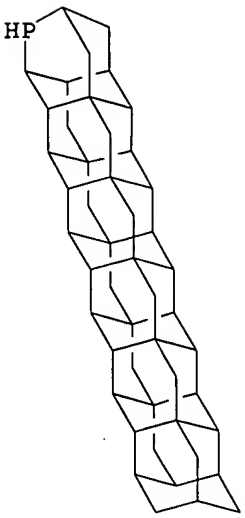

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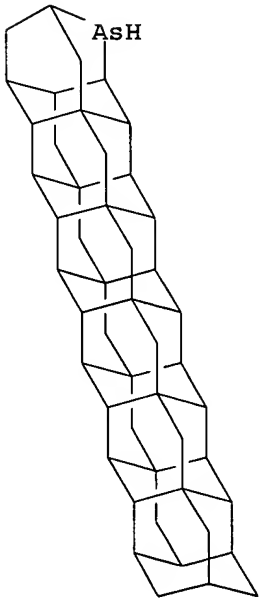

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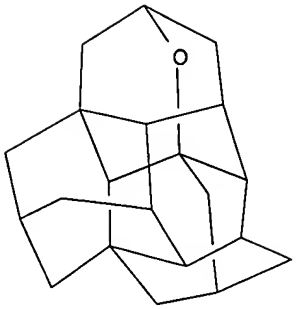

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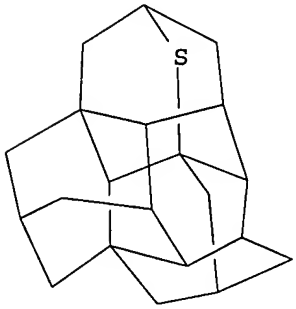

RN 652999-08-1 HCAPLUS
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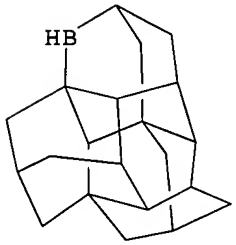

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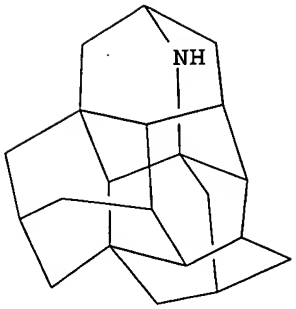

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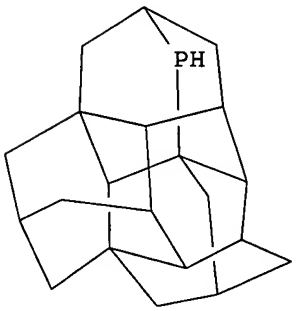

RN 652999-12-7 HCAPLUS
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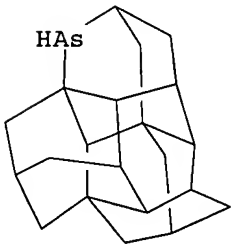

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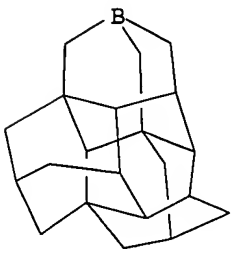
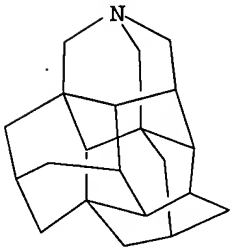
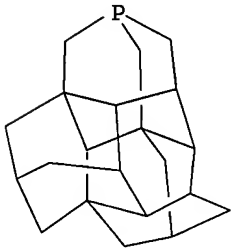


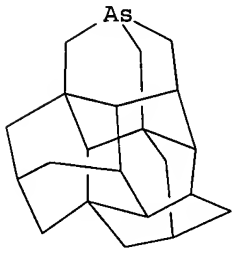
RN 652999-36-5 HCAPLUS
CN 3H,4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenz[de,h]isoquinoline, decahydro- (9CI) (CA INDEX NAME)



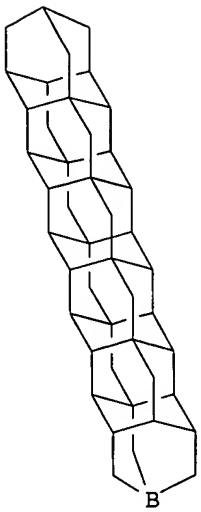
RN 652999-38-7 HCAPLUS
CN 3H,4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenz[de,h]isophosphinoline, decahydro- (9CI) (CA INDEX NAME)



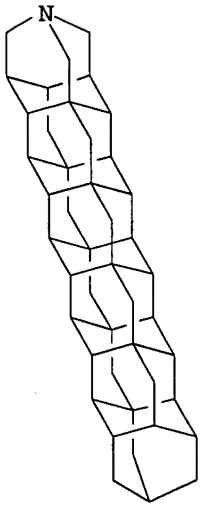
RN 652999-39-8 HCAPLUS
CN 3H,4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenz[de,h]isoarsinoline, decahydro- (9CI) (CA INDEX NAME)



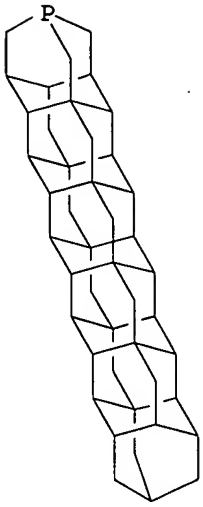
RN 652999-40-1 HCAPLUS
CN [121212121] Boradecamantane (9CI) (CA INDEX NAME)



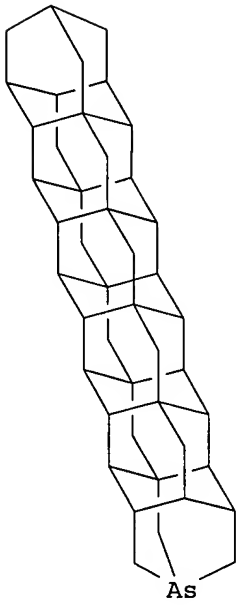
RN 652999-41-2 HCAPLUS
CN [121212121] Azadecamantane (9CI) (CA INDEX NAME)



RN 652999-42-3 HCAPLUS
CN [121212121] Phosphadecamantane (9CI) (CA INDEX NAME)

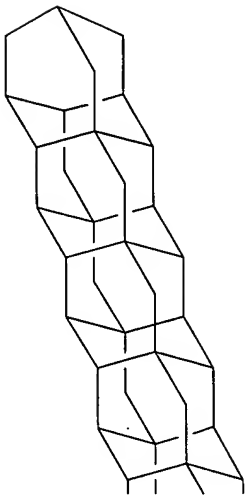


RN 652999-43-4 HCAPLUS
CN [121212121] Arsadecamantane (9CI) (CA INDEX NAME)

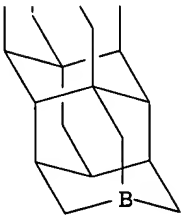


RN 652999-44-5 HCAPLUS
CN [1212121212] Boraundecamantane (9CI) (CA INDEX NAME)

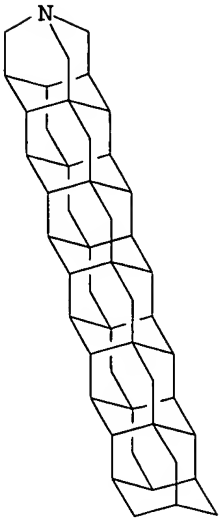
PAGE 1-A



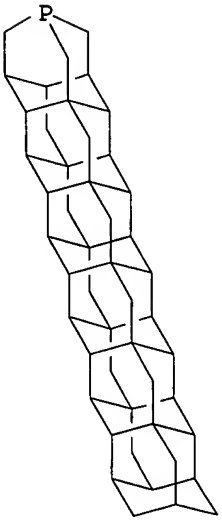
PAGE 2-A



RN 652999-45-6 HCAPLUS
CN [1212121212] Azaundecamantane (9CI) (CA INDEX NAME)

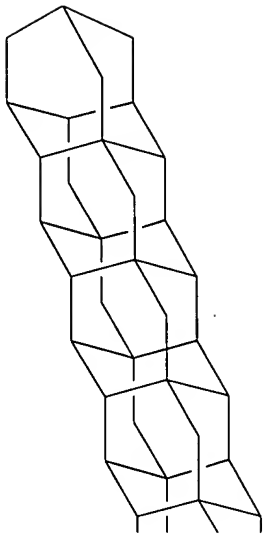


RN 652999-46-7 HCAPLUS
CN [1212121212] Phosphaundecamantane (9CI) (CA INDEX NAME)

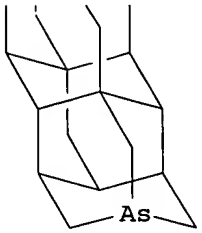


RN 652999-47-8 HCAPLUS
CN [1212121212] Arsaundecamantane (9CI) (CA INDEX NAME)

PAGE 1-A



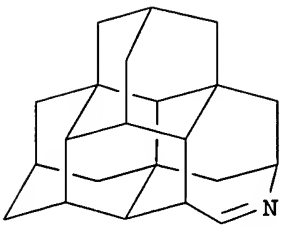
PAGE 2-A



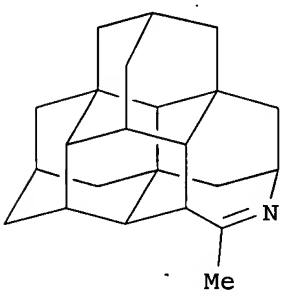
IT **652999-16-1P 652999-17-2P 652999-18-3P**
652999-19-4P 652999-20-7P 652999-23-0P
652999-24-1P 652999-25-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)

RN 652999-16-1 HCAPLUS

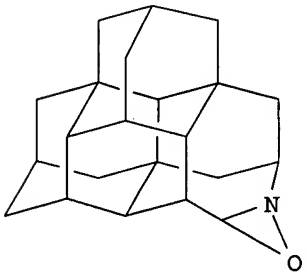
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylideneanthra[9,1-cd]azepine, 3,4,6,7,7a,8a,9,10,11,12a,12b,12c-dodecahydro- (9CI) (CA INDEX NAME)



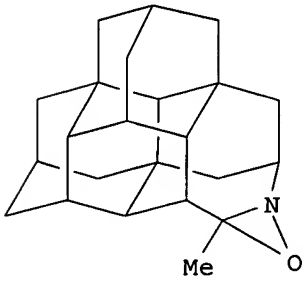
RN 652999-17-2 HCAPLUS
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylideneanthra[9,1-cd]azepine, 3,4,6,7,7a,8a,9,10,11,12a,12b,12c-dodecahydro-1-methyl- (9CI) (CA INDEX NAME)



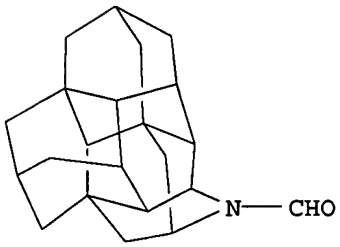
RN 652999-18-3 HCAPLUS
CN 8H,9H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-5H-anthra[9,1-cd]oxazirino[2,3-a]azepine, dodecahydro- (9CI) (CA INDEX NAME)



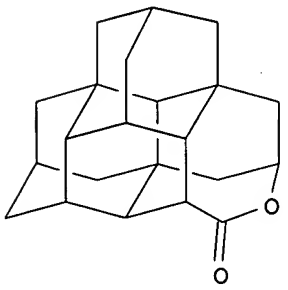
RN 652999-19-4 HCAPLUS
CN 8H,9H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-5H-anthra[9,1-cd]oxazirino[2,3-a]azepine, dodecahydro-12c-methyl- (9CI) (CA INDEX NAME)



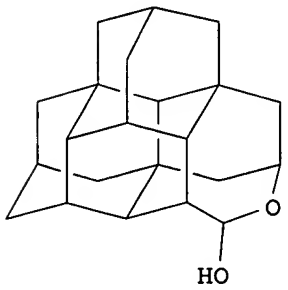
RN 652999-20-7 HCAPLUS
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenzo[de,h]quinoline-1-carboxaldehyde, dodecahydro- (9CI) (CA INDEX NAME)



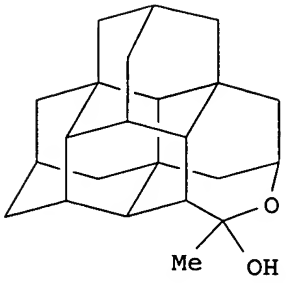
RN 652999-23-0 HCAPLUS
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-one, dodecahydro- (9CI) (CA INDEX NAME)



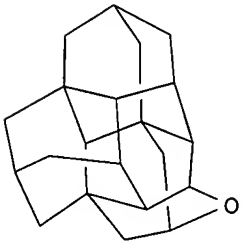
RN 652999-24-1 HCAPLUS
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-ol, dodecahydro- (9CI) (CA INDEX NAME)



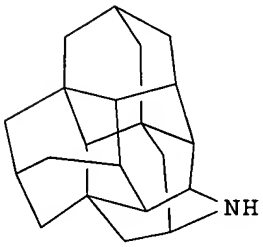
RN 652999-25-2 HCAPLUS
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-ol, dodecahydro-1-methyl- (9CI) (CA INDEX NAME)



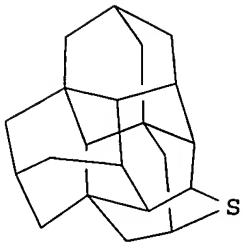
IT **652999-15-0P 652999-21-8P 652999-32-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)
RN 652999-15-0 HCAPLUS
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]pyran, dodecahydro- (9CI) (CA INDEX NAME)



RN 652999-21-8 HCAPLUS
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenzo[de,h]quinoline, dodecahydro- (9CI) (CA INDEX NAME)



RN 652999-32-1 HCAPLUS
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]thiopyran, dodecahydro- (9CI) (CA INDEX NAME)



L64 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:800853 HCAPLUS
DN 140:339373
ED Entered STN: 13 Oct 2003
TI Theoretical analysis of a carbon-carbon dimer placement tool for diamond mechanosynthesis
AU Merkle, Ralph C.; Freitas, Robert A., Jr.
CS Zyvex Corp., Richardson, TX, USA
SO Journal of Nanoscience and Nanotechnology (2003), 3(4), 319-324
CODEN: JNNOAR; ISSN: 1533-4880
PB American Scientific Publishers
DT Journal
LA English
CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 24
AB D. functional theory is used with Gaussian 98 to analyze a new family of proposed mechanosynthetic tools that could be employed for the placement of two carbon atoms-a carbon-carbon (CC) dimer-on a growing diamond surface at a specific site. Optimized structures and potential energies were calculated for 5,5'-ethynediyl-bridged 2,2',4,4',9,9'-**biadamantane** and its 5,5'-disila-, 5,5'-digerma-, 5,5'-distanna-, 5,5'-diplumba- and 5-sila-5-germa-analogs. The stationary points for the 5,5'-ethynediyl-, 5,5'-ethylidyne carbene and 2,2',4,4',5,5',9,9'-**biadamantanes** were located. The anal. focuses on specific Group IV-substituted **biadamantane** tool tip structures and evaluates their stability and the strength of the bond they make with the CC dimer. These tools should be stable in a vacuum and should be able to hold and position a CC dimer in a manner suitable for positionally controlled diamond mechanosynthesis at room temperature
ST **biadamantane** sila germa stanna plumba ethynediyl DFT geometry energy; carbon dimer placement tool **biadamantane** alkyne geometry potential energy; polycyclic compd condensed **adamantane** **biadamantane** heterocycle ethynediyl DFT calcn; heterocyclic compd silicon germanium tin lead polycyclic DFT energy; DFT geometry energy polycyclic **adamantane** Group IVA deriv calcn; diamond **diamondoid** hydrocarbon **diadamantane** hetero substituted DFT geometry energy; mol structure optimized hetero **diadamantane** ethynediyl linked
IT Density functional theory
(B3LYP; geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
IT Potential energy
(DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
IT Carbenes (methylene derivatives)
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer

precursors)
IT Bond energy
(carbon-heteroatom bond energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
IT Dimers
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(carbon; DFT geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
IT Hydrocarbons, properties
RL: PRP (Properties)
(**diamondoid**, **biadamantanes**; DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
IT Group IVA element compounds
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(**heterobiadamantanes**; DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
IT Molecular structure
(optimized; of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
IT Polycyclic compounds
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(tricyclic; DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
IT 681029-73-2P **681029-74-3P** **681029-75-4P**
681029-76-5P **681029-77-6P**
RL: BYP (Byproduct); PRP (Properties); PREP (Preparation)
(DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
IT 681029-78-7, [4,6]Fulleroid-C20 **681029-79-8**, Disila[4,6]fulleroid-C20 **681029-80-1**, Digerma[4,6]fulleroid-C20 **681029-81-2**, Distanna[4,6]fulleroid-C20 **681029-82-3**, Diplumba[4,6]fulleroid-C20 **681029-83-4**, Germasila[4,6]fulleroid-C20
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
IT 681029-67-4 **681029-68-5** **681029-69-6**
681029-70-9 **681029-71-0** **681029-72-1**
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(fragmentation; DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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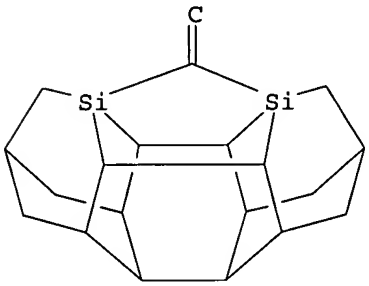
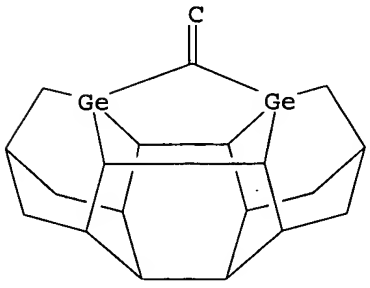
IT **681029-74-3P 681029-75-4P 681029-76-5P 681029-77-6P**
RL: BYP (Byproduct); PRP (Properties); PREP (Preparation)
(DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)

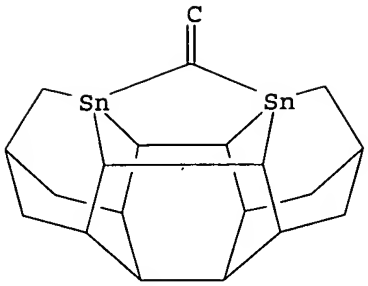
RN 681029-74-3 HCAPLUS
CN Methylene, disila[5,6]fulleroid-C21-ylidene- (9CI) (CA INDEX NAME)



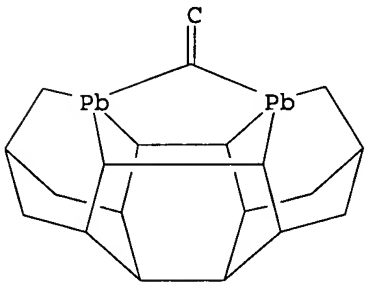
RN 681029-75-4 HCAPLUS
CN Methylene, digerma[5,6]fulleroid-C21-ylidene- (9CI) (CA INDEX NAME)



RN 681029-76-5 HCAPLUS
CN Methylene, distanna[5,6]fulleroid-C21-ylidene- (9CI) (CA INDEX NAME)

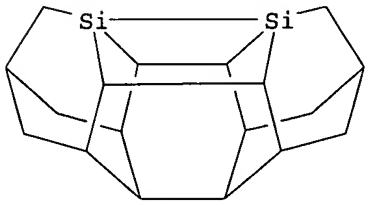


RN 681029-77-6 HCAPLUS
CN Methylene, diplumba[5,6]fulleroid-C21-ylidene- (9CI) (CA INDEX NAME)

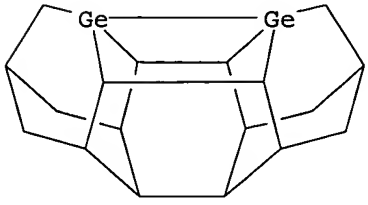


IT **681029-79-8**, Disila[4,6]fulleroid-C20 **681029-80-1**, Digerma[4,6]fulleroid-C20 **681029-81-2**, Distanna[4,6]fulleroid-C20 **681029-82-3**, Diplumba[4,6]fulleroid-C20 **681029-83-4**, Germasila[4,6]fulleroid-C20
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)

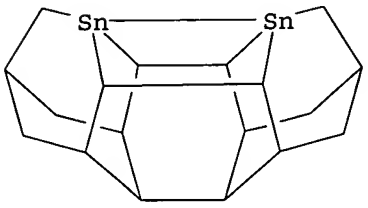
RN 681029-79-8 HCAPLUS
CN Disila[4,6]fulleroid-C20 (9CI) (CA INDEX NAME)



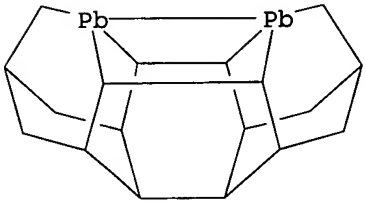
RN 681029-80-1 HCAPLUS
CN Digerma[4,6]fulleroid-C20 (9CI) (CA INDEX NAME)



RN 681029-81-2 HCAPLUS
CN Distanna[4,6]fulleroid-C20 (9CI) (CA INDEX NAME)



RN 681029-82-3 HCAPLUS
CN Diplumba[4,6]fulleroid-C20 (9CI) (CA INDEX NAME)



RN 681029-83-4 HCAPLUS
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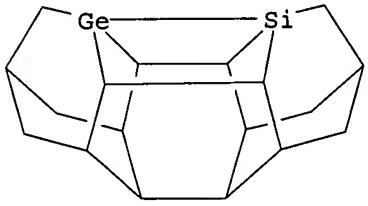
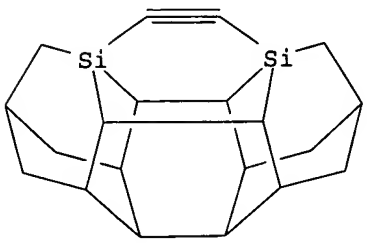
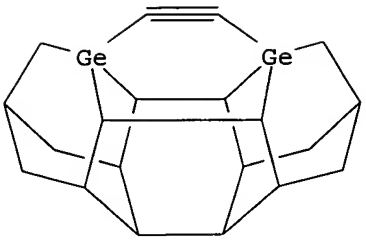


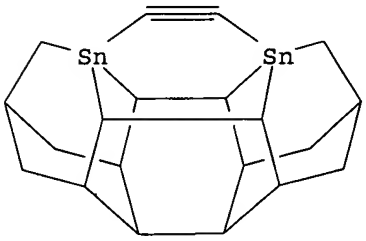
IT **681029-68-5 681029-69-6 681029-70-9**
681029-71-0 681029-72-1
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(fragmentation; DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
RN 681029-68-5 HCAPLUS
CN Disila[6]fulleroid-C22, tetradehydro- (9CI) (CA INDEX NAME)



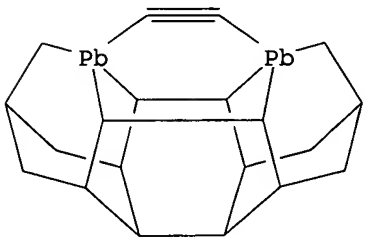
RN 681029-69-6 HCAPLUS
CN Digerma[6]fulleroid-C22, tetradehydro- (9CI) (CA INDEX NAME)



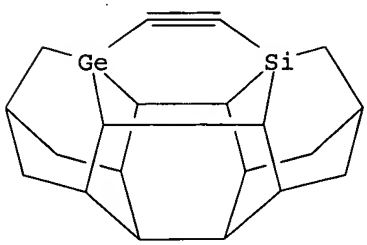
RN 681029-70-9 HCAPLUS
CN Distanna[6]fulleroid-C22, tetradehydro- (9CI) (CA INDEX NAME)



RN 681029-71-0 HCAPLUS
CN Diplumba[6]fulleroid-C22, tetradehydro- (9CI) (CA INDEX NAME)



RN 681029-72-1 HCAPLUS
CN Germasila[6]fulleroid-C22, tetradehydro- (9CI) (CA INDEX NAME)



=> fil reg
FILE 'REGISTRY' ENTERED AT 10:24:18 ON 10 MAR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 MAR 2005 HIGHEST RN 844817-50-1
DICTIONARY FILE UPDATES: 9 MAR 2005 HIGHEST RN 844817-50-1

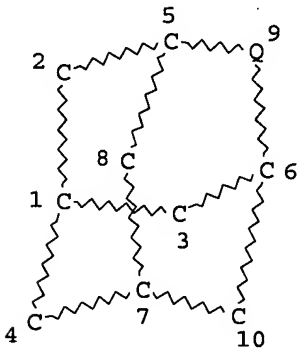
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

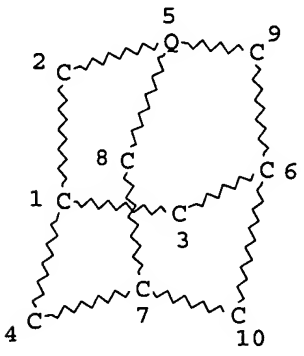
=> => d sta que l57
L47 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L49 STR



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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE
L51             STR
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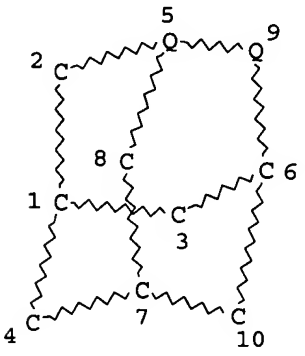


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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE
L56             SCR 1845
L57           0 SEA FILE=REGISTRY SSS SAM (L47 OR L49 OR L51) AND L56

  3.7% PROCESSED   1000 ITERATIONS                              0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       524526 TO   544074
PROJECTED ANSWERS:               0 TO        0



=> => fil reg
FILE 'REGISTRY' ENTERED AT 07:00:49 ON 14 MAR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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provided by InfoChem.

STRUCTURE FILE UPDATES:   13 MAR 2005  HIGHEST RN 845467-46-1
DICTIONARY FILE UPDATES:  13 MAR 2005  HIGHEST RN 845467-46-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
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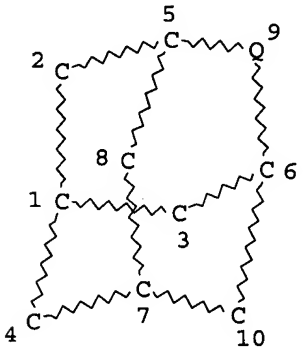
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

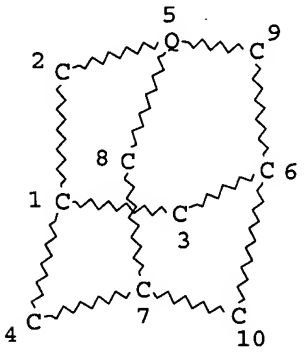
=> d sta que l5
L1 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

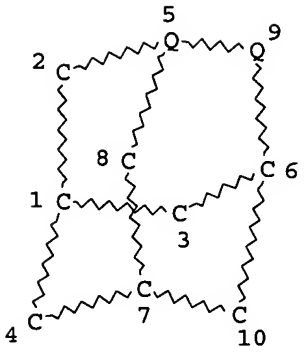
STEREO ATTRIBUTES: NONE
L2 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L3 STR

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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE
L4              SCR 1845
L5          125 SEA FILE=REGISTRY SSS FUL (L1 OR L2 OR L3) AND L4

100.0% PROCESSED 537537 ITERATIONS                          125 ANSWERS
SEARCH TIME: 00.00.09


=> d his

     (FILE 'HOME' ENTERED AT 06:40:19 ON 14 MAR 2005)
               SET COST OFF

     FILE 'REGISTRY' ENTERED AT 06:40:32 ON 14 MAR 2005
               ACT SHIAO622A/A
              ---------
L1             STR
L2             STR
L3             STR
L4             SCR 1845
L5          125 SEA FILE=REGISTRY SSS FUL (L1 OR L2 OR L3) AND L4
              ---------
               ACT SHIAO622/A
              ---------
L6   (         77)SEA FILE=HCAPLUS ABB=ON  PLU=ON  ?TETRAMANTAN? OR ?TRIAMANTAN?
L7   (        263)SEA FILE=HCAPLUS ABB=ON  PLU=ON  ?DIAMONDOID?
L8   (         37)SEA FILE=HCAPLUS ABB=ON  PLU=ON  L7 AND L6
L9   (         98)SEA FILE=HCAPLUS ABB=ON  PLU=ON  L7 AND ?AMANTAN?
L10  (         98)SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L8 OR L9)
L11               SEL  PLU=ON  L10 1- RN :     796 TERMS
L12  (        796)SEA FILE=REGISTRY ABB=ON  PLU=ON  L11
L13  (        401)SEA FILE=REGISTRY ABB=ON  PLU=ON  L12 AND NR>=5
L14  (        359)SEA FILE=REGISTRY ABB=ON  PLU=ON  L13 NOT HYDROCARBON
L15  (         80)SEA FILE=REGISTRY ABB=ON  PLU=ON  L14 AND ?AMANTAN?/CNS
L16  (         59)SEA FILE=REGISTRY ABB=ON  PLU=ON  L15 NOT C6-C6-C6/ES
L17  (         38)SEA FILE=REGISTRY ABB=ON  PLU=ON  L16 AND (SE OR AS OR B OR AL
L18  (         16)SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 AND (C15H20O2 OR C16H20O4
L19  (         22)SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 NOT L18
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```
L20 (        42)SEA FILE=REGISTRY ABB=ON  PLU=ON  L15 NOT L17
L21 (       279)SEA FILE=REGISTRY ABB=ON  PLU=ON  L14 NOT (L15 OR L16 OR L17 OR
L22 (        24)SEA FILE=REGISTRY ABB=ON  PLU=ON  L21 AND (C18H24GE2 OR C21H27P
L23 (        29)SEA FILE=REGISTRY ABB=ON  PLU=ON  L21 AND (C21H26S3 OR C23H30O2
L24 (        40)SEA FILE=REGISTRY ABB=ON  PLU=ON  (L22 OR L23)
L25 (         5)SEA FILE=REGISTRY ABB=ON  PLU=ON  L24 AND (CARBOXYLIC OR C21H26
L26 (         2)SEA FILE=REGISTRY ABB=ON  PLU=ON  (652999-05-8/BI OR 652999-15-
L27 (         3)SEA FILE=REGISTRY ABB=ON  PLU=ON  L25 NOT L26
L28 (        37)SEA FILE=REGISTRY ABB=ON  PLU=ON  L24 NOT L27
L29          59 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L19 OR L28)
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L30          75 S L5 NOT L29
L31          15 S L30 AND (C21H14S OR C21H17P OR C21H15P OR C21H15N OR C21H14S3
L32          50 S L29 AND L5
L33           1 S L5 AND C21H24B2
L34          16 S L31,L33
                SAV L34 SHIAO622B/A
L35           9 S L29 NOT L32
                E 2395/RID
L36          19 S E6-E29
                E 99573/RID
L37          10 S E3-E13
                E 81072/RID
L38           4 S E3-E8
                E 7965/RID
L39          54 S E3-E56
L40          25 S L39 NOT L29,L32,L34
L41           7 S L40 AND (CU OR SI)/ELS
L42          33 S L34,L37,L41
L43          26 S L42 NOT L29
L44           7 S L29 AND L42
                SAV L43 SHIAO622C/A

     FILE 'HCAOLD' ENTERED AT 06:57:56 ON 14 MAR 2005
L45           0 S L29
L46           0 S L43

     FILE 'HCAPLUS' ENTERED AT 06:58:01 ON 14 MAR 2005
L47           8 S L43
L48           1 S L47 AND (LIU S? OR CARLSON R? OR DAHL J?)/AU
L49           1 S L47 AND CHEVRO?/PA,CS
L50           1 S L48,L49
L51           8 S L47,L50

     FILE 'USPATFULL' ENTERED AT 07:00:33 ON 14 MAR 2005
L52           1 S L43

     FILE 'REGISTRY' ENTERED AT 07:00:49 ON 14 MAR 2005

=> d ide can tot l43

L43  ANSWER 1 OF 26  REGISTRY  COPYRIGHT 2005 ACS on STN
RN   656230-43-2  REGISTRY
CN   8H,9H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-5H-
     anthra[9,1-cd]oxazirino[2,3-a]azepine (9CI)  (CA INDEX NAME)
MF   C22 H15 N O
CI   RPS
SR   CA Index Guide or Ring Systems Handbook
```
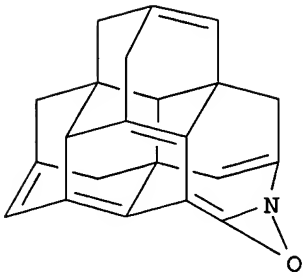
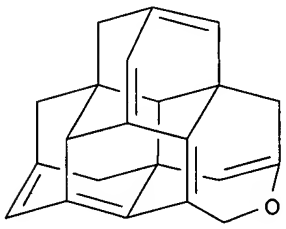
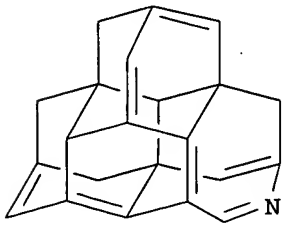



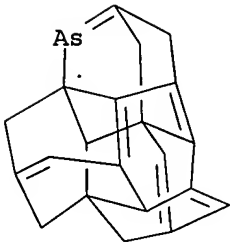
L43 ANSWER 2 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-41-0 REGISTRY
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin (9CI) (CA INDEX NAME)
MF C22 H16 O
CI RPS
SR CA Index Guide or Ring Systems Handbook



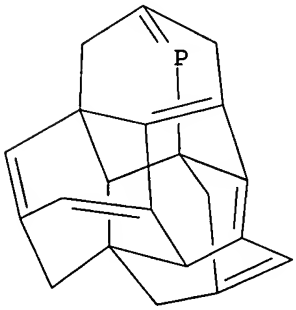
L43 ANSWER 3 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-40-9 REGISTRY
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylideneanthra[9,1-cd]azepine (9CI) (CA INDEX NAME)
MF C22 H15 N
CI RPS
SR CA Index Guide or Ring Systems Handbook



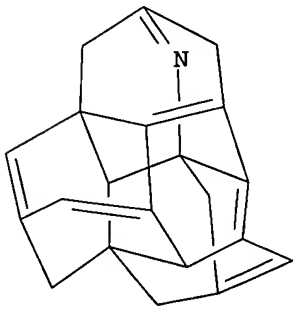
L43 ANSWER 4 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-39-6 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-naphth[1,2,3-de]arsinoline (9CI) (CA INDEX NAME)
MF **C21 H15 As**
CI RPS
SR CA Index Guide or Ring Systems Handbook



L43 ANSWER 5 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-38-5 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-naphtho[1,2,3-de]phosphinoline (9CI) (CA INDEX NAME)
MF **C21 H15 P**
CI RPS
SR CA Index Guide or Ring Systems Handbook



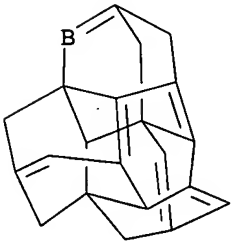
L43 ANSWER 6 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-37-4 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-naphtho[1,2,3-de]quinoline (9CI) (CA INDEX NAME)
MF **C21 H15 N**
CI RPS
SR CA Index Guide or Ring Systems Handbook



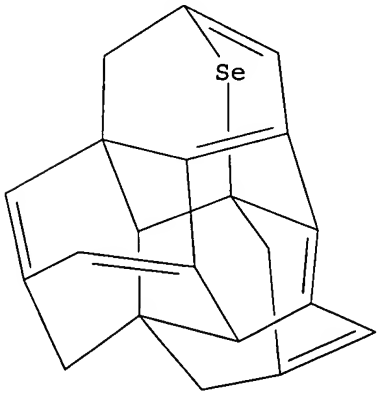
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L43 ANSWER 7 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-36-3 REGISTRY

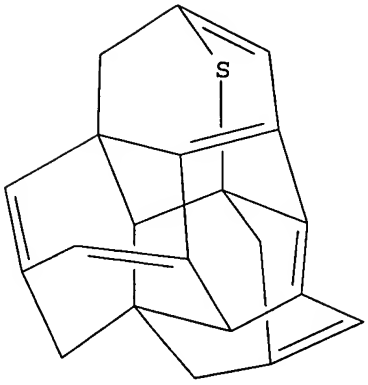
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-anthra[1,9-bc]borin (9CI) (CA INDEX NAME)
MF **C21 H15 B**
CI RPS
SR CA Index Guide or Ring Systems Handbook



L43 ANSWER 8 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-35-2 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-bc]selenin (9CI) (CA INDEX NAME)
MF **C21 H14 Se**
CI RPS
SR CA Index Guide or Ring Systems Handbook

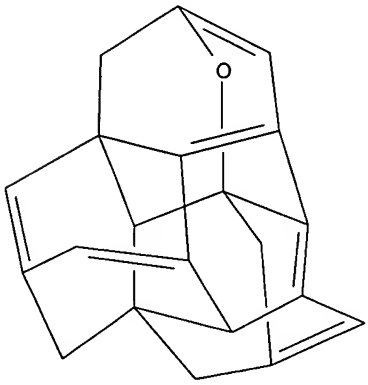


L43 ANSWER 9 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-34-1 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-bc]thiopyran (9CI) (CA INDEX NAME)
MF **C21 H14 S**
CI RPS
SR CA Index Guide or Ring Systems Handbook



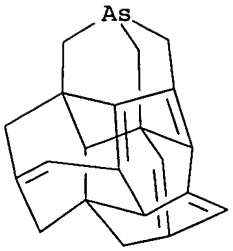
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L43 ANSWER 10 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-33-0 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-bc]pyran (9CI) (CA INDEX NAME)
MF **C21 H14 O**
CI RPS
SR CA Index Guide or Ring Systems Handbook

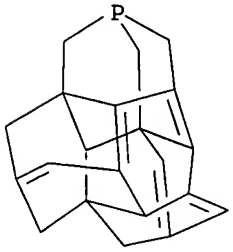


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

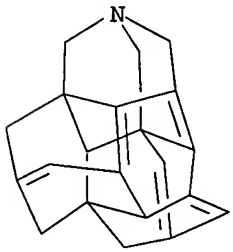
L43 ANSWER 11 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-32-9 REGISTRY
CN 3H,4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenz[de,h]isoarsinoline (9CI) (CA INDEX NAME)
MF **C21 H17 As**
CI RPS
SR CA Index Guide or Ring Systems Handbook



L43 ANSWER 12 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-31-8 REGISTRY
CN 3H,4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenz[de,h]isophosphinoline (9CI) (CA INDEX NAME)
MF **C21 H17 P**
CI RPS
SR CA Index Guide or Ring Systems Handbook



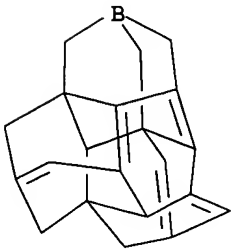
L43 ANSWER 13 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-30-7 REGISTRY
CN 3H,4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenz[de,h]isoquinoline (9CI) (CA INDEX NAME)
MF **C21 H17 N**
CI RPS
SR CA Index Guide or Ring Systems Handbook



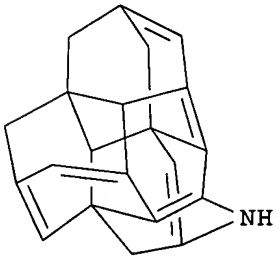
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L43 ANSWER 14 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-29-4 REGISTRY
CN 3H,4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-anthra[1,9-cd]borin (9CI) (CA INDEX NAME)
MF **C21 H17 B**

CI RPS
SR CA Index Guide or Ring Systems Handbook

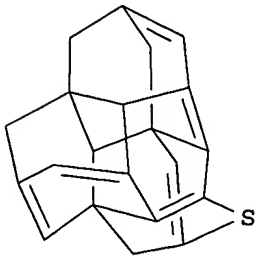


L43 ANSWER 15 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-28-3 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenzo[de,h]quinoline (9CI) (CA INDEX NAME)
MF **C21 H15 N**
CI RPS
SR CA Index Guide or Ring Systems Handbook



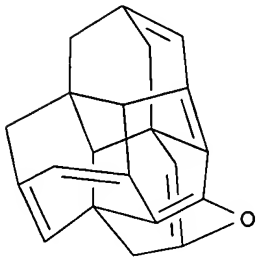
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L43 ANSWER 16 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-27-2 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]thiopyran (9CI) (CA INDEX NAME)
MF **C21 H14 S**
CI RPS
SR CA Index Guide or Ring Systems Handbook



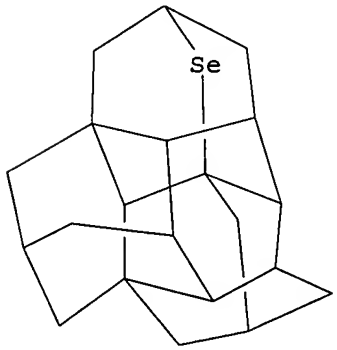
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L43 ANSWER 17 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-26-1 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]pyran (9CI) (CA INDEX NAME)
MF **C21 H14 O**
CI RPS
SR CA Index Guide or Ring Systems Handbook



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L43 ANSWER 18 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 652999-07-0 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-bc]selenin, dodecahydro- (9CI) (CA INDEX NAME)
MF **C21 H26 Se**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PRP (Properties)



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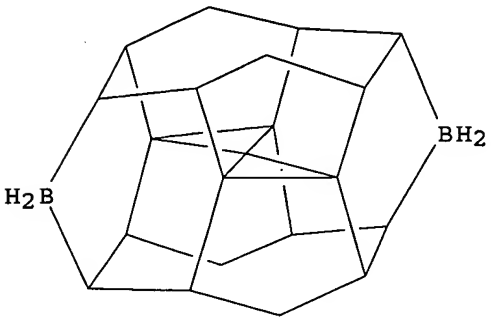
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:146009

L43 ANSWER 19 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 475276-89-2 REGISTRY
CN 1,2:16,20-Diborylene-4,9,14,18-methyno-1,2:6,7:11,12:16,20-tetraseco[5]fullerane-C20-Ih, 21,23-dihydro- (9CI) (CA INDEX NAME)

MF **C21 H24 B2**
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:370137

L43 ANSWER 20 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 142381-39-3 REGISTRY
CN Phosphonium, tetraphenyl-, nonakis[μ-(ethanethiolato)]tetrakis[μ3-(ethanethiolato)]tris[(ethanethiolato)indate]hexacuprate(1-) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Cuprate(1-), nonakis[μ-(ethanethiolato)]tetrakis[μ3-(ethanethiolato)]tris[(ethanethiolato)indate]hexa-, tetraphenylphosphonium (9CI)
MF **C32 H80 Cu6 In3 S16 . C24 H20 P**
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

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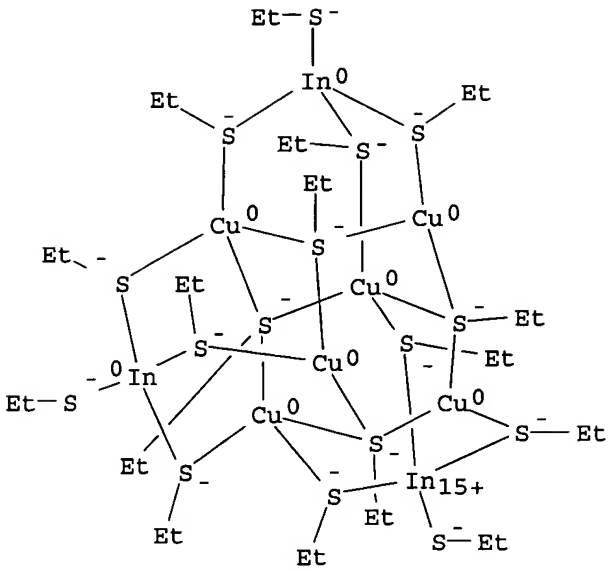
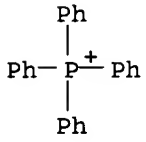
CRN 142381-38-2
CMF C32 H80 Cu6 In3 S16
CCI CCS



CM 2

CRN 18198-39-5
CMF C24 H20 P



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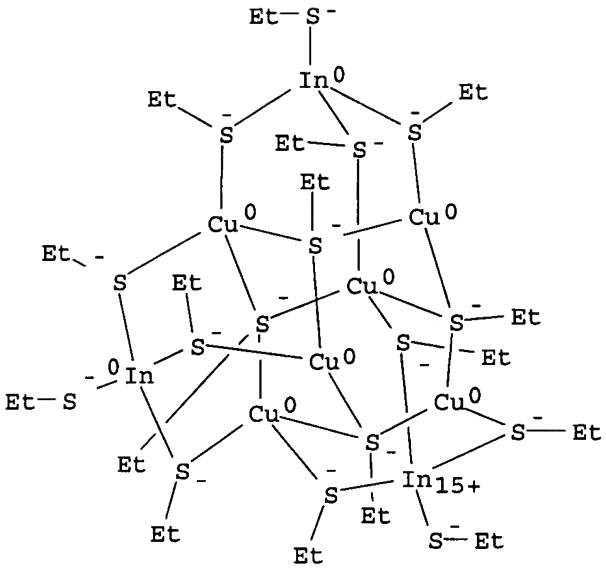
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 117:61532

L43 ANSWER 21 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 142381-38-2 REGISTRY
CN Cuprate(1-), nonakis[μ-(ethanethiolato)]tetrakis[μ3-(ethanethiolato)]tris[(ethanethiolato)indate]hexa- (9CI) (CA INDEX NAME)
MF **C32 H80 Cu6 In3 S16**
CI CCS, COM
SR CA



L43 ANSWER 22 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 121472-96-6 REGISTRY
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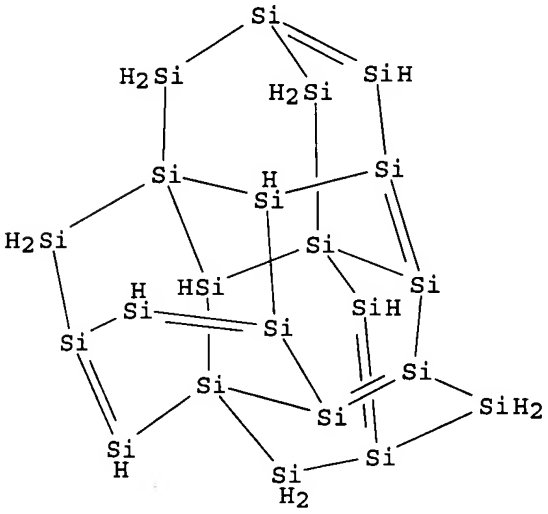
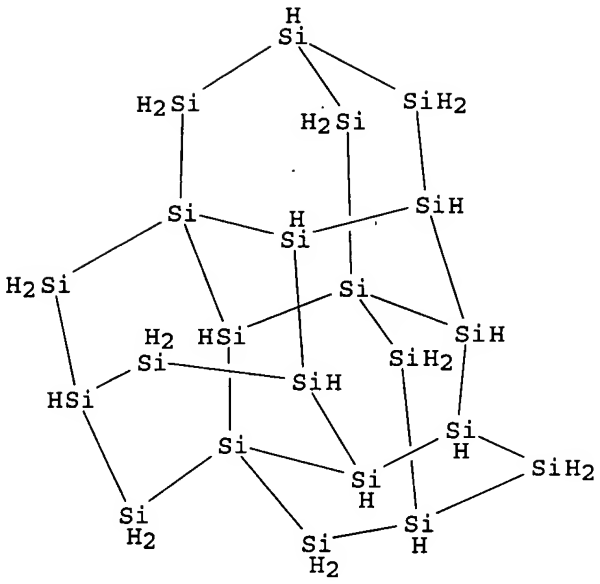
MF **H16 Si22**
CI RPS
SR CA Index Guide or Ring Systems Handbook



L43 ANSWER 23 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 119052-10-7 REGISTRY
CN 4H,7H-2,11:5,13-Disilano-9,7,3a,11-[1,2]trisilanediyl[3]ylidene-1H-heptadecasilabenz[de]anthracene, dodecahydro- (9CI) (CA INDEX NAME)
MF **H28 Si22**
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)



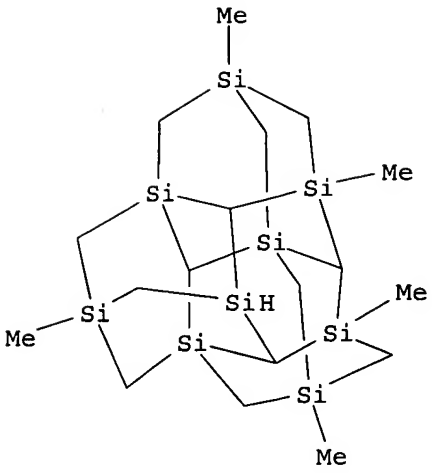
3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:173087

REFERENCE 2: 135:10213

REFERENCE 3: 110:86206

L43 ANSWER 24 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 94396-97-1 REGISTRY
CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-2,5,6a,7a,9-pentamethyl- (9CI) (CA INDEX NAME)
MF **C18 H38 Si9**
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



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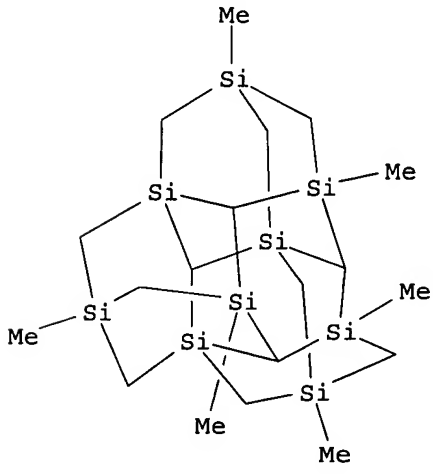
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 102:78938

L43 ANSWER 25 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 31714-54-2 REGISTRY
CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-2,5,6a,7a,9,11b-hexamethyl- (8CI, 9CI) (CA INDEX NAME)
MF **C19 H40 Si9**
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



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2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 102:78938

REFERENCE 2: 73:56178

L43 ANSWER 26 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 29861-92-5 REGISTRY
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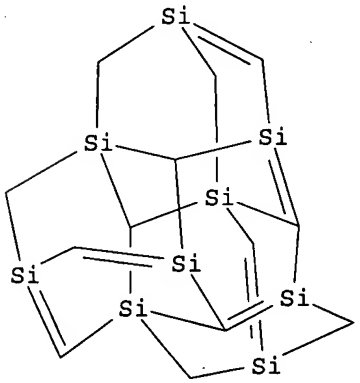
CI RPS



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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 10 Mar 2005 (20050310/PD)
FILE LAST UPDATED: 10 Mar 2005 (20050310/ED)
HIGHEST GRANTED PATENT NUMBER: US6865747
HIGHEST APPLICATION PUBLICATION NUMBER: US2005055750
CA INDEXING IS CURRENT THROUGH 10 Mar 2005 (20050310/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 10 Mar 2005 (20050310/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2005

>>> USPAT2 is now available. USPATFULL contains full text of the <<<
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>>> applications. USPAT2 contains full text of the latest US <<<
>>> publications, starting in 2001, for the inventions covered in <<<
>>> USPATFULL. A USPATFULL record contains not only the original <<<
>>> published document but also a list of any subsequent <<<
>>> publications. The publication number, patent kind code, and <<<
>>> publication date for all the US publications for an invention <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc. <<<

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>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<

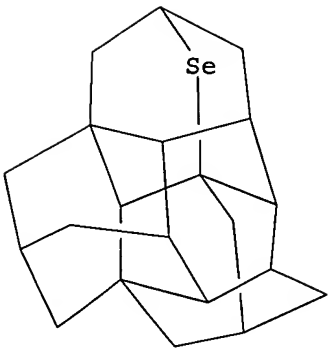
>>> the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> => d bib abs hitstr l52

L52 ANSWER 1 OF 1 USPATFULL on STN
AN 2004:77366 USPATFULL
TI Heterodiamondoids
IN Liu, Shenggao, Hercules, CA, UNITED STATES
Carlson, Robert M., Petaluma, CA, UNITED STATES
Dahl, Jeremy E., Palo Alto, CA, UNITED STATES
PA CHEVRON USA INC. (U.S. corporation)
PI US 2004059145 A1 20040325
AI US 2003-622130 A1 20030716 (10)
PRAI US 2002-397367P 20020718 (60)
DT Utility
FS APPLICATION
LREP William H. Benz, BURNS, DOANE, SWECKER & MATHIS, L.L.P., P.O. Box 1404, Alexandria, VA, 22313-1404
CLMN Number of Claims: 37
ECL Exemplary Claim: 1
DRWN 51 Drawing Page(s)
LN.CNT 2469
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB This invention is related to heteroatom containing diamondoids (i.e., "heterodiamondoids") which are compounds having a diamondoid nucleus in which one or more of the diamondoid nucleus carbons has been substitutionally replaced with a noncarbon atom. These heteroatom substituents impart desirable properties to the diamondoid. In addition, the heterodiamondoids are functionalized affording compounds carrying one or more functional groups covalently pendant therefrom. This invention is further related to polymerizable functionalized heterodiamondoids. In a preferred aspect of this invention the diamondoid nuclei are triamantane and higher diamondoid nuclei. In another preferred aspect, the heteroatoms are selected to give rise to diamondoid materials which can serve as n- and p-type materials in electronic devices can serve as optically active materials.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **652999-07-0**
(calcn. of heat of formation; preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)
RN 652999-07-0 USPATFULL
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-bc]selenin, dodecahydro- (9CI) (CA INDEX NAME)

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FILE COVERS 1907 - 14 Mar 2005  VOL 142 ISS 12
FILE LAST UPDATED: 13 Mar 2005  (20050313/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> d all hitstr tot l51

L51  ANSWER 1 OF 8  HCAPLUS  COPYRIGHT 2005 ACS on STN
AN   2004:80675  HCAPLUS
DN   140:146009
ED   Entered STN:  01 Feb 2004
TI   Preparation of heterodiamondoids from fused adamantanes
IN   Liu, Shenggao; Carlson, Robert M.
PA   Chevron U.S.A. Inc., USA; Dahl, Jeremy E.
SO   PCT Int. Appl., 134 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
IC   ICM  C07D311-78
     ICS  C07D313-06; C07D335-04; C07D221-18
CC   27-16 (Heterocyclic Compounds (One Hetero Atom))
     Section cross-reference(s): 76
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
     --------------      ----   --------    --------------------    --------
PI   WO 2004009577        A1    20040129    WO 2003-US22483         20030717
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

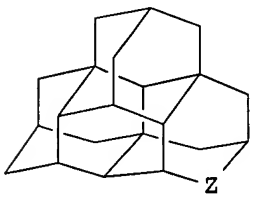
US 2004059145 A1 20040325 US 2003-622130 20030716
PRAI US 2002-397367P P 20020718
US 2002-397368P P 20020718

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004009577	ICM	C07D311-78
	ICS	C07D313-06; C07D335-04; C07D221-18
US 2004059145	ECLA	C07C023/20; C07C049/423; C07C049/617; C07C061/29; C07D221/22; C07D311/96; C07D313/06; C07D335/04; C07D471/10+221C+221C+9; C07F009/6568C

OS MARPAT 140:146009

GI



I

AB This invention is related to heteroatom containing diamondoids (i.e., 'heterodiamondoids'), e.g. azatetramantane, oxatetramantane, and thiatetramantane (I; X = NH, O, S), which are compds. having a diamondoid nucleus in which one or more of the diamondoid nucleus carbons has been substitutionally replaced with a noncarbon atom. These heteroatom substituents impart desirable properties to the diamondoid. In addition, the heterodiamondoids are functionalized affording compds. carrying one or more functional groups covalently pendant therefrom. This invention is further related to polymerizable functionalized heterodiamondoids. In a preferred aspect of this invention the diamondoid nuclei are triamantane and higher diamondoid nuclei. In another preferred aspect, the heteroatoms are selected to give rise to diamondoid materials which can serve as n- and p-type materials in electronic devices and in optical devices as optically active materials (no data).

ST heterodiamondoid prepn; azatetramantane oxatetramantane thiatetramantane prepn

IT Formation enthalpy
(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

IT Heterocyclic compounds
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

IT 652998-89-5, [121212121] Decamantane 652998-90-8, [121212121] Oxadecamantane 652998-91-9, [121212121] Thiadecamantane 652998-92-0, [121212121] Selenadecamantane 652998-93-1, [121212121] Boradecamantane 652998-94-2, [121212121] Azadecamantane 652998-95-3, [121212121] Phosphadecamantane 652998-96-4, [121212121] Arsadecamantane

652998-97-5, [1212121212] Undecamantane 652998-98-6, [1212121212] Oxaundecamantane 652998-99-7, [1212121212] Thiaundecamantane 652999-00-3, [1212121212] Selenaundecamantane 652999-01-4, [1212121212] Boraundecamantane 652999-02-5, [1212121212] Azaundecamantane 652999-03-6, [1212121212] Phosphaundecamantane 652999-04-7, [1212121212] Arsaundecamantane 652999-05-8 652999-06-9 **652999-07-0** 652999-08-1 652999-09-2 652999-11-6 652999-12-7 652999-35-4 652999-36-5 652999-38-7 652999-39-8 652999-40-1, [121212121] Boradecamantane 652999-41-2, [121212121] Azadecamantane 652999-42-3, [121212121] Phosphadecamantane 652999-43-4, [121212121] Arsadecamantane 652999-44-5, [1212121212] Boraundecamantane 652999-45-6, [1212121212] Azaundecamantane 652999-46-7, [1212121212] Phosphaundecamantane 652999-47-8, [1212121212] Arsaundecamantane
RL: PRP (Properties)
(calcn. of heat of formation; preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

IT 917-54-4, Methyllithium 27745-90-0 73635-95-7 73635-96-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

IT 546101-72-8P 546102-13-0P 652999-13-8P 652999-14-9P 652999-16-1P 652999-17-2P 652999-18-3P 652999-19-4P 652999-20-7P 652999-23-0P 652999-24-1P 652999-25-2P 652999-26-3P 652999-27-4P 652999-29-6P 652999-30-9P 652999-31-0P 652999-33-2P 652999-34-3P 653570-14-0P 653570-15-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

IT 652999-15-0P 652999-21-8P 652999-22-9P 652999-28-5P 652999-32-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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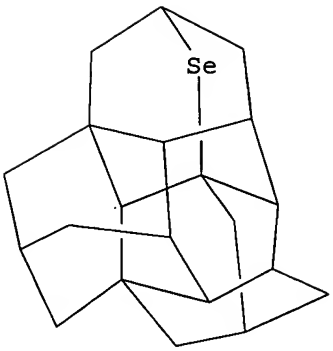
IT **652999-07-0**
RL: PRP (Properties)
(calcn. of heat of formation; preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

RN 652999-07-0 HCAPLUS

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-bc]selenin, dodecahydro- (9CI) (CA INDEX NAME)



L51 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:685440 HCAPLUS
DN 137:370137
ED Entered STN: 11 Sep 2002
TI The Theoretical Design of Neutral Planar Tetracoordinate Carbon Molecules with C(C)4 Substructures
AU Wang, Zhi-Xiang; Schleyer, Paul von Rague
CS Computational Chemistry Annex, University of Georgia, Athens, GA, 30602-2525, USA
SO Journal of the American Chemical Society (2002), 124(40), 11979-11982
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
CC 29-4 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 24
AB Using a new charge-compensation strategy, neutral mols. were designed with perfectly planar C(C)4-type tetracoordinate carbon arrangements (ptC) employing DFT computations. These designs, based on the planar preference of methane dications, replace two remote carbons in spiroalkaplanes by borons or two remote hydrogens by BH3 groups; the two formally anionic boron units which result compensate the formal double pos. charge on the central ptC's. The LUMOs correspond to the "wasted" lone pair HOMOs of the alkaplanes. As compared to the latter, π occupancies on the central carbon are much smaller (less than 0.7e), and the IPs are much larger. The newly predicted compds. utilize all of the electrons more effectively. There are no lone pairs, and the ptC-C bond lengths are ca. 1.50 Å. The Wiberg bond index sums of the ptC's are near 3.2, and the boron sums are close to 4.
ST planar tetracoordinate carbon boron compd DFT; mol electronic structure spiroalkaplane boron compd DFT; HOMO planar tetracoordinate carbon boron compd DFT
IT Molecular structure
(optimized; theor. study of tetracoordinate carbon mols. with C(C)4 substructures)
IT Stereochemistry
(tetrahedral vs. planar; theor. study of tetracoordinate carbon mols. with C(C)4 substructures)
IT Density functional theory
Electronic structure
HOMO (molecular orbital)
Stabilization energy
(theor. study of tetracoordinate carbon mols. with C(C)4 substructures)
IT 74-82-8, Methane, properties 157-40-4, Spiropentane 20741-88-2, Methane(1+), properties 73353-64-7, Indeno[7,1-cd]indene 101517-28-6, Spiro[2.2]pentane, radical ion(1+) 148810-14-4, Methane, radical

ion(2+), properties 179032-57-6, Spiro[2.2]octaplane 251918-68-0
330597-93-8 475276-87-0 475276-88-1 **475276-89-2**
475276-90-5 475276-91-6 475276-92-7 475276-93-8 475276-94-9
475276-95-0 475276-96-1 475276-97-2 475276-98-3 475467-16-4
475467-22-2
RL: PRP (Properties)
(theor. study of tetracoordinate carbon mols. with C(C)4 substructures)

RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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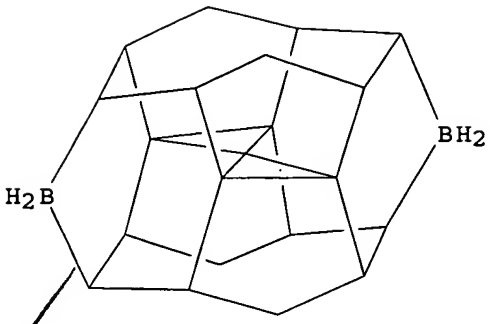
IT **475276-89-2**
RL: PRP (Properties)
(theor. study of tetracoordinate carbon mols. with C(C)4 substructures)

RN 475276-89-2 HCAPLUS

CN 1,2:16,20-Diborylene-4,9,14,18-methyno-1,2:6,7:11,12:16,20-tetraseco[5]fullerane-C20-Ih, 21,23-dihydro- (9CI) (CA INDEX NAME)



L51 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:892659 HCAPLUS
DN 136:173087
ED Entered STN: 12 Dec 2001
TI Size, Order, and Dimensional Relations for Silicon Cluster Polarizabilities
AU Jansik, B.; Schimmelpfennig, B.; Norman, P.; Mochizuki, Y.; Luo, Y.; Aagren, H.
CS Theoretical Chemistry, Royal Institute of Technology, Stockholm, S-106 91, Swed.
SO Journal of Physical Chemistry A (2002), 106(2), 395-399
CODEN: JPCAFH; ISSN: 1089-5639
PB American Chemical Society
DT Journal
LA English
CC 65-5 (General Physical Chemistry)
AB Response theory calcns. in the RPA are applied to linear polarizabilities and second hyperpolarizabilities of 1-, 2-, and 3-dimensional hydrogen-terminated silicon clusters. Successive enlargement of the clusters to embody on the order of 50 silicon atoms plus bond-saturating hydrogen atoms allows for extrapolation to bulk values of individual silicon atom contributions in the 1D and 3D cases. Modern effective core potentials are shown to provide excellent approxns. to the all-electron values in all cases; errors for both polarizabilities and hyperpolarizabilities are on the order of 1%. The findings indicate considerable time savings in predictions of the elec. polarizability properties of elements beyond the first row atoms.
ST silicon cluster hydrogen termination polarizability hyperpolarizability response theory RPA; effective core potential silicon cluster hydrogen termination polarizability hyperpolarizability
IT Basis sets
(effective core potential; in study of polarizabilities and hyperpolarizabilities of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by response theory in RPA)
IT Electron correlation
(in study of polarizabilities and hyperpolarizabilities of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by response theory in RPA)
IT Cluster structure
Hyperpolarizability
Polarizability
(of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by response theory in RPA)
IT Clusters
Size effect
(polarizabilities and hyperpolarizabilities of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by

response theory in RPA)
IT Silanes
RL: PRP (Properties)
(polarizabilities and hyperpolarizabilities of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by response theory in RPA)
IT 291-59-8, Cyclohexasilane 1590-87-0, Silicon hydride (Si2H6) 7783-26-8, Silicon hydride (Si3H8) 7783-29-1, Silicon hydride (Si4H10) 14693-61-9, Hexasilane 39517-09-4, Octasilane 41518-75-6, Decasilane 72244-91-8, Tetradecasilane 94570-81-7, Triacontasilane 99759-72-5, Hexasilabenzene **119052-10-7** 128171-51-7, Eicosasilane 133754-37-7, Hexadecasilane 153549-12-3, Pentadecasilane 155101-73-8, Tricyclo[3.3.1.13,7]decasilane 209683-92-1, Dodecasilane 226714-57-4 334939-73-0, Silicon hydride (Si35H36) 340809-92-9 397250-81-6, Dopentacontasilane 397250-82-7, Hexadecasilapyrene 397250-83-8, Tetracosasilacoronene 397250-84-9 397250-85-0, Silicon hydride (Si54H56)
RL: PRP (Properties)
(polarizabilities and hyperpolarizabilities of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by response theory in RPA)
RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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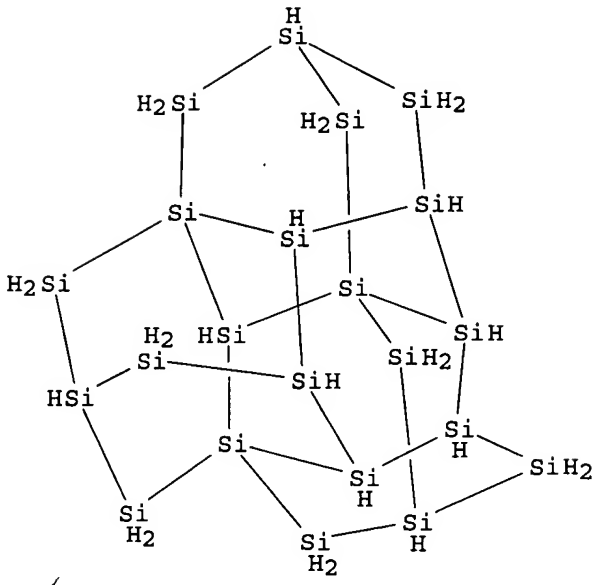
IT **119052-10-7**
RL: PRP (Properties)
(polarizabilities and hyperpolarizabilities of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by response theory in RPA)
RN 119052-10-7 HCAPLUS
CN 4H,7H-2,11:5,13-Disilano-9,7,3a,11-[1,2]trisilanediyl[3]ylidene-1H-heptadecasilabenz[de]anthracene, dodecahydro- (9CI) (CA INDEX NAME)



L51 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:207328 HCAPLUS
DN 135:10213
ED Entered STN: 22 Mar 2001
TI Polarizability of silicon clusters
AU Mochizuki, Y.; Agren, H.
CS CCSE, Japan Atomic Energy Research Institute, Meguro-ku, Tokyo, 153-0061, Japan
SO Chemical Physics Letters (2001), 336(5,6), 451-456
CODEN: CHPLBC; ISSN: 0009-2614
PB Elsevier Science B.V.
DT Journal
LA English
CC 65-5 (General Physical Chemistry)
Section cross-reference(s): 76
AB The polarizability of hydrogen-terminated silicon clusters derived from the silicon diamond-lattice structure was evaluated by linear response calcns. The dependences on cluster size and basis set were systematically investigated. A convergence in calculated polarizability per silicon atom toward the bulk value was found. Frequency-dependent polarizabilities were also addressed.
ST polarizability silicon cluster
IT Cluster structure
Polarizability
(polarizability of silicon clusters)
IT 291-59-8, Cyclohexasilane 7440-21-3, Silicon, properties
119052-10-7 147207-30-5, Silicon hydride (Si35H36)
212783-55-6, Silicon hydride (Si5H) 226714-57-4 312613-06-2, Silicon hydride (Si10H16) 340809-92-9
RL: PRP (Properties)
(polarizability of silicon clusters)
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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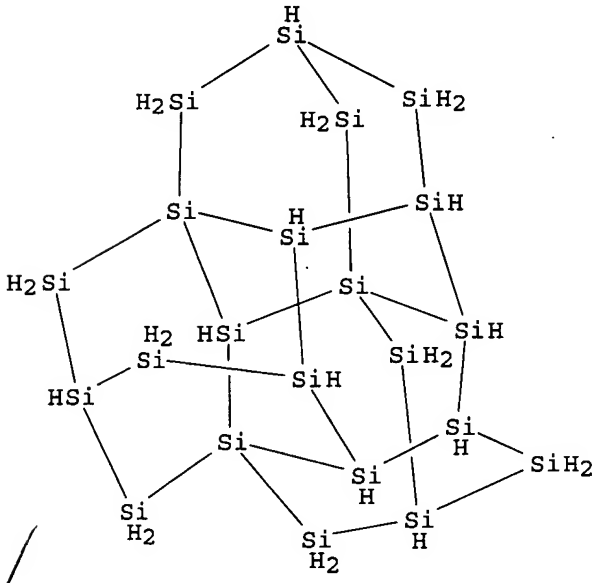
(20) Woon, D; J Chem Phys 1993, V98, P1358 HCAPLUS

IT **119052-10-7**
RL: PRP (Properties)
(polarizability of silicon clusters)

RN 119052-10-7 HCAPLUS

CN 4H,7H-2,11:5,13-Disilano-9,7,3a,11-[1,2]trisilanediyl[3]ylidene-1H-heptadecasilabenz[de]anthracene, dodecahydro- (9CI) (CA INDEX NAME)



L51 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1992:461532 HCAPLUS
DN 117:61532
ED Entered STN: 08 Aug 1992

TI Synthesis and structure of the first indium-copper cluster, [Cu6In3(SEt)16]- and its possible relevance to CuInS2

AU Hirpo, Wakgari; Dhingra, Sandeep; Kanatzidis, Mercouri G.
CS Cent. Fundam. Mater. Res., Michigan State Univ., East Lansing, MI, 48824, USA

SO Journal of the Chemical Society, Chemical Communications (1992), (7), 557-9
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75

AB (Ph4P)[Cu6In3(SEt)16] was prepared by the reaction of [Cu(MeCN)4]PF6 with (Ph4P)[In(SEt)4] and its crystal structure shows an adamantoid framework.

ST crystal structure copper indium ethanethiolato cluster; thiolato copper indium nonanuclear cluster

IT Crystal structure
Molecular structure
(of copper indium ethanethiolato nonanuclear cluster)

IT Cluster compounds, coordinative
RL: SPN (Synthetic preparation); PREP (Preparation)
(copper-indium-sulfur, ethanethiolato, preparation and crystal structure of)

IT **142381-39-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

IT 142029-65-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with copper acetonitrile complex)

IT 64443-05-6, Tetrakis(acetonitrile)copper(1+) hexafluorophosphate(1-)
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with indate ethanethiolato complex)

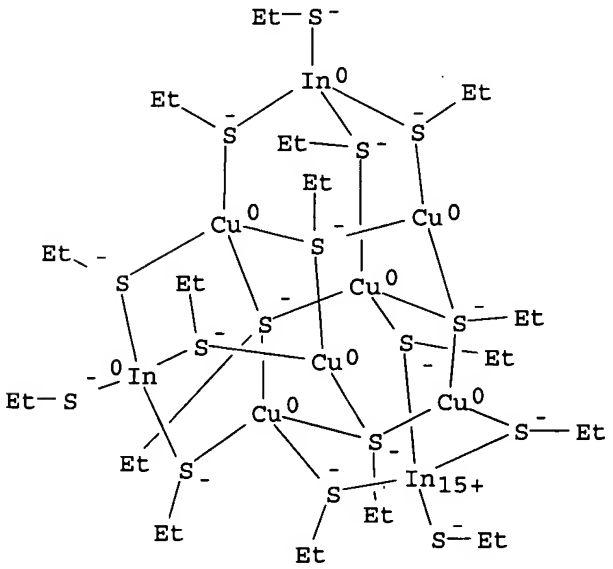
IT **142381-39-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

RN 142381-39-3 HCAPLUS

CN Phosphonium, tetraphenyl-, nonakis[μ-(ethanethiolato)]tetrakis[μ3-(ethanethiolato)]tris[(ethanethiolato)indate]hexacuprate(1-) (9CI) (CA INDEX NAME)

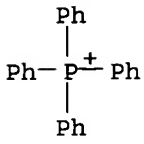
CM 1

CRN 142381-38-2
CMF C32 H80 Cu6 In3 S16
CCI CCS

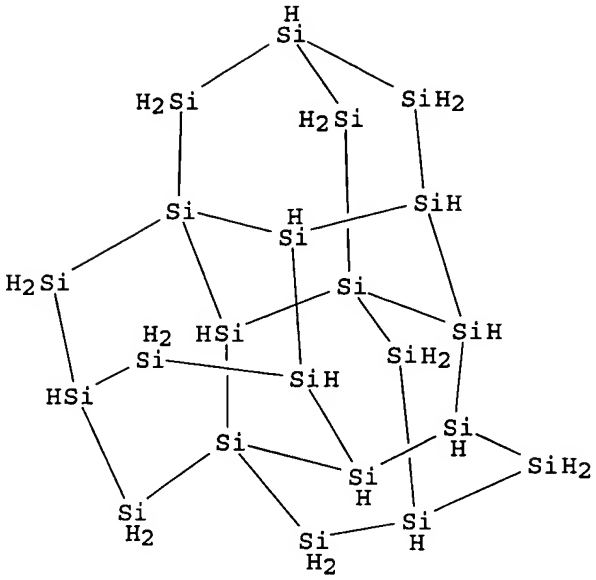


CM 2

CRN 18198-39-5
CMF C24 H20 P



L51 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1989:86206 HCAPLUS
DN 110:86206
ED Entered STN: 04 Mar 1989
TI Hyperfine interactions in cluster models of the Pb defect center
AU Cook, Michael; White, C. T.
CS Nav. Res. Lab., Washington, DC, 20375-5000, USA
SO Physical Review B: Condensed Matter and Materials Physics (1988), 38(14), 9674-85
CODEN: PRBMDO; ISSN: 0163-1829
DT Journal
LA English
CC 76-1 (Electric Phenomena)
AB Hyperfine interactions in the Pb center (denoted schematically as Si3.tplbond.Si.), an electron trap, at the Si(111)/SiO2 interface have been studied with use of spin-polarized self-consistent multiple-scattering Xα calcns. on Si22H21/Si6O18H6 and Si22H27 cluster models. The theor. hyperfine tensor agrees very well with experiment when the trivalent atom Si' is relaxed by a value typical of geometries found for the neutral paramagnetic charge state in semiempirical and ab initio cluster calcns. Spin-polarization effects are very important for a detailed description of the Pb defect, particularly with respect to the hyperfine couplings at nuclei close to the defect atom. The largest such superhyperfine interaction is produced not by the nearest-neighbor atoms as has commonly been assumed, but by 3 second-nearest neighbors located below Si' in the bulk c-Si. The isotropic and anisotropic superhyperfine components and the direction of the principle axes predicted by the present calcns. have been confirmed by recent ESR expts.
ST interface silicon silica hyperfine interaction center
IT Trapping and Traps
(at silicon interface with silicon, cluster model of center for)
IT Interface
(silica-silicon, Pb center hyperfine interaction at, spin-polarized self-consistent multiple-scattering Xα calcn. on)
IT 7440-21-3, Silicon, properties
RL: PRP (Properties)
(defect center hyperfine interaction at interface of silica with)
IT 7631-86-9, Silica, properties
RL: PRP (Properties)
(defect center hyperfine interaction at interface of silicon with)
IT 119052-09-4 **119052-10-7**
RL: PRP (Properties)
(interface defect center hyperfine interaction at silicon-silica interface from cluster model of)
IT **119052-10-7**
RL: PRP (Properties)
(interface defect center hyperfine interaction at silicon-silica interface from cluster model of)
RN 119052-10-7 HCAPLUS
CN 4H,7H-2,11:5,13-Disilano-9,7,3a,11-[1,2]trisilanediyl[3]ylidene-1H-heptadecasilabenz[de]anthracene, dodecahydro- (9CI) (CA INDEX NAME)

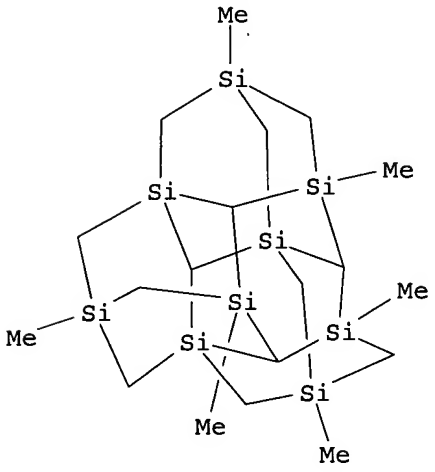


L51 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1985:78938 HCAPLUS
DN 102:78938
ED Entered STN: 09 Mar 1985
TI Formation of organosilicon compounds. 100. Isolation of higher molecular weight carbosilanes from the pyrolysis of tetramethylsilane
AU Fritz, G.; Woerns, K. P.
CS Inst. Anorg. Chem., Univ. Karlsruhe, Karlsruhe, D-7500, Fed. Rep. Ger.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1984), 512, 103-25
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA German
CC 29-6 (Organometallic and Organometalloidal Compounds)
GI

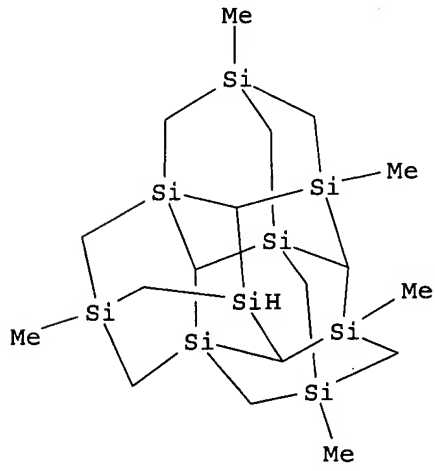
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A systematic investigation of the carbosilanes containing 6 to 9 Si atoms per mol. formed by pyrolysis of SiMe4 was achieved by means of column chromatog. sepns. combined with HPLC. Eleven pure compds. and mixts. of I (R = Me, R1 = CH2SiMe2CH2SiMe3; R = R1 = Me3SiCH2) as well as of II and III were isolated. The predominant structure is that of the carborundanes using only Me and H as Si substituents. Only in compds. IV and V are some of the Si-C 6-membered rings in the chair form. In compds. such as VI another possibility of connecting 1,3,5,7-tetrasilaadamantane frameworks to higher mol. carbosilanes is realized.
ST silane tetramethyl pyrolysis; pyrolysis methylsilane; polycyclic carbosilane; silane silaadamantane poly
IT Chromatography, column and liquid
(high-performance, isolation of high mol. weight carbosilanes from the pyrolysis of tetramethylsilane by)
IT 26393-20-4P **31714-54-2P** 94396-94-8P 94396-95-9P
94396-96-0P **94396-97-1P** 94396-98-2P 94396-99-3P
94397-00-9P
RL: PREP (Preparation)
(isolation of, from pyrolysis of tetramethylsilane)

IT 50938-70-0P 65000-98-8P 86932-03-8P 94396-90-4P 94396-91-5P
94396-92-6P 94396-93-7P 94411-13-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by pyrolysis of tetramethylsilane)
IT 75-76-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(pyrolysis of, isolation of higher mol. weight carbosilanes from)
IT **31714-54-2P 94396-97-1P**
RL: PREP (Preparation)
(isolation of, from pyrolysis of tetramethylsilane)
RN 31714-54-2 HCAPLUS
CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-2,5,6a,7a,9,11b-hexamethyl- (8CI, 9CI) (CA INDEX NAME)

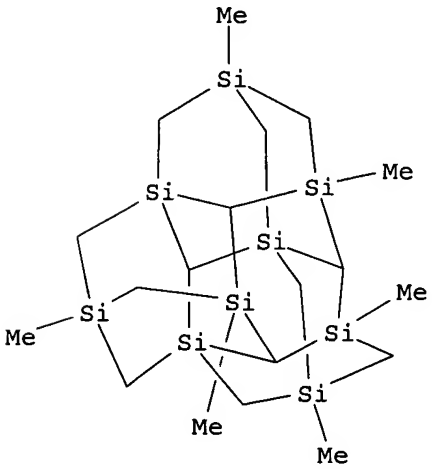


RN 94396-97-1 HCAPLUS
CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-2,5,6a,7a,9-pentamethyl- (9CI) (CA INDEX NAME)



L51 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1970:456178 HCAPLUS

DN 73:56178
ED Entered STN: 12 May 1984
TI Silicon-carbon compounds with a carborundum structure ("carborundanes")
AU Fritz, Gerhard; Diem, Fritz; Koehler, Helmut; Kummer, Dieter; Scheer, Heinz
CS Inst. Anorg. Chem., Univ. Karlsruhe, Karlsruhe, Fed. Rep. Ger.
SO Angewandte Chemie, International Edition in English (1970), 9(6), 464-5
CODEN: ACIEAY; ISSN: 0570-0833
DT Journal
LA English
CC 29 (Organometallic and Organometalloidal Compounds)
GI For diagram(s), see printed CA Issue.
AB 1,3,5,7-Tetramethyl-1,3,5,7-tetrasilatricyclo [3.3.1.13,7]decane (I) and small amts. 1,3,7,9,11,13-hexamethyl-1,3,5,7,9,11,13-heptasilahexacyclo [7.5.1.13,13.17,11.05,12.05,15]heptadecane (II), 3,7,11,13,15,17-hexamethyl-1,3,5,7,9,11,13,15,17-enneasilaenneacyclo [9.1.7.11,5.13,17.17,15.05,16.09,14.09,20.013,18] docosane (III), and 3,7,11,17-tetramethyl-1,3,5,7,9,11,13,15,17,19-decasilaundecacyclo [9.9.1.11,5.13.19.15,19.17,15.113,17.09,14.09,22.013,20.015,24]hexacosane (IV) are obtained when SiMe4 is pyrolyzed (700°). NMR data for II-IV are given.
ST carborundanes silicon carbon compds; silicon carbon compds carborundanes; carbon silicon compds carborundanes; silaadamantanes; adamantanes sila; methyl silanes pyrolysis; silanes methyl pyrolysis; pyrolysis methyl silanes
IT 26393-20-4P **31714-54-2P** 32069-85-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **31714-54-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 31714-54-2 HCAPLUS
CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-2,5,6a,7a,9,11b-hexamethyl- (8CI, 9CI) (CA INDEX NAME)



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